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The Total Least Squares Problem

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1. Introduction

The total least squares method is one of several linear parameter estimation techniques that have been devised to compensate for data errors. The basic motivation for *total least squares* (TLS) is the following: Let a set of multidimensional data points (vectors) be given. How can one obtain a linear model that explains these data? The idea is to modify all data points in such a way that some norm of the modification is minimized subject to the constraint that the modified vectors satisfy a linear relation.

The origin of this basic idea can be traced back to the beginning of this century. It was rediscovered many times, often independently, mainly in the statistical and psychometric literature. However, it is only in the last decade that the technique also found wide use in scientific and engineering applications. One of the main reasons for its popularity is the availability of efficient and numerical robust algorithms, in which the *singular value decomposition* plays a prominent role. Another reason is the fact that TLS is an *application oriented* procedure. It is ideally suited for situations in which all data are corrupted by noise, which is almost always the case in engineering applications. In this sense it is a powerful extension of the classical least squares method, which corresponds only to a partial modification of the data.

1.1. A simple example

The problem of *linear parameter estimation* arises in a broad class of scientific disciplines such as signal processing, automatic control, system theory and in general engineering, statistics, physics, economics, biology, medicine, etc. ... It starts from a model described by a linear equation,

$$\alpha_1 x_1 + \cdots + \alpha_n x_n = \beta \,, \tag{1}$$

where $\alpha_1, \ldots, \alpha_n$ and β denote the variables and $x = [x_1, \ldots, x_n]^T \in \mathbb{R}^n$ plays

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the role of a parameter vector that characterizes the specific system. The basic problem is then to determine an estimate of the *true* but *unknown* parameters from certain measurements of the variables. This gives rise to an *over-determined* set of m linear equations ($m > n$):

$$Ax \approx b\,, \tag{2}$$

where the i-th row of the data matrix $A \in \mathbb{R}^{m \times n}$ and the vector of observations $b \in \mathbb{R}^m$ contain the measurements of the variables $\alpha_1, \ldots, \alpha_n$ and β, respectively.

In the classical least squares (LS) approach the measurements A of the variables α_i (the left-hand side of (2)) are assumed to be free of error and hence, all errors are confined to the observation vector b (the right-hand side of (2)). However, this assumption is frequently unrealistic: sampling errors, human errors, modeling errors and instrument errors may imply inaccuracies of the data matrix A as well. TLS is one method of fitting that is appropriate when there are errors in *both* the observation vector b and the data matrix A. If gives the 'best' estimates (in a statistical sense) when all variables are subject to independently and identically distributed errors with zero mean and common covariance matrix equal to the identity matrix, up to a scaling factor. Several other and more general approaches to this problem have led to many other fitting techniques for the linear as well as for the nonlinear cases, see e.g., [23, 18, 35, 46, 50, 54].

To illustrate the effect of the use of TLS in comparison with LS, we consider here a simple example of parameter estimation: only one parameter ($n = 1$) is to be estimated. Hence, equation (1) reduces to

$$\alpha x = \beta\,. \tag{3}$$

An estimate for parameter x is to be found from m measurements of the variables α and β:

$$\begin{aligned} a_i &= a_i^0 + \Delta a_i \\ & \qquad\qquad , i = 1, \ldots, m \\ b_i &= b_i^0 + \Delta b_i \end{aligned} \tag{4}$$

by solving the linear system (2) with $A = [a_1, \ldots, a_m]^{\mathrm{T}}$ and $b = [b_1, \ldots, b_m]^{\mathrm{T}}$. Δa_i and Δb_i represent the random errors added to the true values a_i^0 and b_i^0 of the variables α and β.

If α can be observed exactly, i.e., $\Delta a_i = 0$, errors only occur in the measurements of β contained in the right-hand side vector b. Hence, the use of LS for solving (2) is appropriate. This method perturbs the observation vector b by a minimum amount r so that $b - r$ can be predicted by Ax. This is done by minimizing the sum of squared differences $\Sigma_{i=1}^{m} (b_i - a_i x)^2$. The best

estimate x' of x follows then immediately:

$$x' = \frac{\sum_{i=1}^{m} a_i b_i}{\sum_{i=1}^{m} a_i^2} . \tag{5}$$

This LS estimation has a nice geometric interpretation as is shown in Figure 1(a).

If β can be measured without error, i.e., $\Delta b_i = 0$, the use of LS is again appropriate. Indeed we can rewrite (3) as

$$\frac{\beta}{x} = \alpha \tag{6}$$

and confine all errors to the measurements of α contained in the right-hand side vector A of the corresponding set of equations $bx^{-1} \approx A$. By minimizing the sum of squared differences between the measured values a_i and the

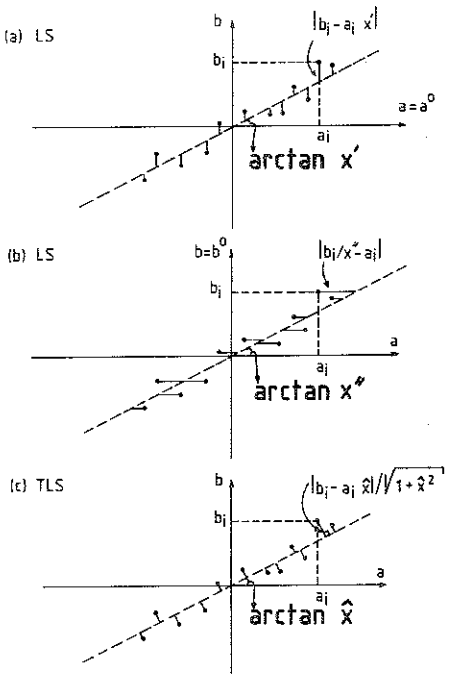


Fig. 1. Geometric interpretation of one-parameter estimation $\alpha x = \beta$ with errors in (a) the measurements b_i of β only (LS solution), (b) the measurements a_i of α only (LS solution), and (c) both the measurements a_i of α and b_i of β (TLS solution).

predicted values b_i/x, the best estimate x'' of x is given by (see Figure 1(b))

$$x'' = \frac{\sum_{i=1}^{m} b_i^2}{\sum_{i=1}^{m} a_i b_i}. \tag{7}$$

In many applications, however, *both* variables are measured with errors, i.e., $\Delta a_i \neq 0$ and $\Delta b_i \neq 0$. If the errors are independently and identically distributed with zero mean and common variance σ_v^2, the best estimate $\hat{x}$ is obtained by minimizing the sum of squared distances of the observed points from the fitted line, i.e., $\Sigma_{i=1}^{m} (b_i - a_i x)^2/(1+x^2)$. This is in fact the solution $\hat{x}$ one obtains by solving (2) with the TLS method for $n=1$. Figure 1(c) illustrates the estimation. The deviations are orthogonal to the fitted line: it is the sum of squares of their lengths that is minimized. Therefore this estimation procedure is sometimes also known as *orthogonal regression*.

HISTORICAL REMARKS. Although the name 'total least squares' appeared only recently in the literature [31], this method of fitting is certainly not new and has a long history in the statistical literature, where the method is known as *orthogonal* regression or *errors-in-variables regression*. Indeed, the univariate line fitting problem ($n=1$) was already discussed in the previous century [5]. Some well-known contributors are Adcock [5], Pearson [43], Koopmans [37], Madansky [40] and York [78] (see [8] for a list of references). The method of orthogonal regression has been rediscovered many times, often independently. About twenty years ago, the technique was extended to multivariate problems ($n>1$) and later to multidimensional problems which deal with more than one observation vector b in (2), e.g., [54, 26].

More recently, the TLS approach to fitting has also stimulated interests outside statistics. In the field of *numerical analysis*, this problem was first studied by Golub and Van Loan [27, 31]. Their analysis, as well as their algorithm, is strongly based on the *singular value decomposition* (SVD). Geometrical insight into the properties of the SVD brought Staar [55] independently to the same concept. Van Huffel and Vandewalle [66] *generalized* the algorithm of Golub and Van Loan to all cases in which their algorithm fails to produce a solution, described the properties of these so-called nongeneric TLS problems and proved that the proposed generalization still satisfies the TLS criteria if additional constraints are imposed on the solution space (see Section 3.2). This seemingly different linear algebraic approach is actually equivalent to the method of multivariate errors-in-variables regression analysis, studied by Gleser [26]. Gleser's method is based on an eigenvalue–eigenvector analysis, while the TLS method uses the SVD which is numerically more robust in the sense of algorithmic implementation. Furthermore, the TLS algorithm computes the minimum norm solution whenever the TLS problem lacks a unique minimizer. These extensions are not considered by Gleser.

In the field of *experimental modal analysis*, the TLS technique (more commonly known as the H_v technique), was also studied recently [38]. And in the field of *system identification*, Levin [39] first studied the same problem. His method, called the *eigenvector method* or *Koopmans–Levin method* [22], computes the same estimate as the TLS algorithm whenever the TLS problem has a unique solution.

NOTATION. The following notation will be used throughout the presentation:

The superscript T denotes the *transpose* of a vector or matrix.

$R(S)$ (resp., $N(S)$) denotes the *column* (resp., *null*) space of a matrix S.

A special notation is convenient for *diagonal* matrices. If A is an $m \times n$ matrix and we write

$$A = \operatorname{diag}(\alpha_1, \ldots, \alpha_p), \quad p = \min\{m, n\},$$

then $a_{ij} = 0$ whenever $i \neq j$ and $a_{ii} = \alpha_i$ for $i = 1, \ldots, p$.

The $m \times m$ *identity* matrix is denoted by I_m or, more simply, by I.

The *set of m linear equations* in n unknowns x is represented in matrix form by

$$Ax \approx b, \tag{8}$$

A is the $m \times n$ data matrix and b is the m-dimensional vector of observations. Unless stated otherwise, we *assume* that the set of equations $Ax \approx b$ is *overdetermined*, i.e., $m > n$, and that all *preprocessing* measures on the data (such as scaling, whitening, centering, standardizing, . . .) have been performed in advance.

$\|M\|_F$ (respectively, $\|M\|_2$) denotes the *Frobenius* norm (respectively, spectrum norm) of a matrix M.

1.2. Problem formulation

In this section we formulate the *main principle* of the TLS problem. A good way to introduce and motivate the method is to recast the *ordinary least squares* (LS) problem [32, Section 5.3; 12].

DEFINITION 1 (*The ordinary least squares problem*). Given an overdetermined set of m linear equations $Ax \approx b$ in n unknowns x. The least squares (LS) problem is the following:

$$\min_{b' \in \mathbb{R}^m} \|b - b'\|_2 \tag{9}$$

$$\text{subject to} \quad b' \in R(A). \tag{10}$$

Once a minimizing b' is found, then any x satisfying

$$Ax = b' \tag{11}$$

is called a LS solution and $\Delta b' = b - b'$ the corresponding LS correction.

Equations (9) and (10) are satisfied if b' is the orthogonal projection of b onto $R(A)$. Thus, the LS problem amounts to perturbing the observation vector b by a minimum amount $\Delta b'$ so that $b' = b - \Delta b'$ can be 'predicted' by the columns of A.

The underlying assumption here is that errors *only* occur in the vector b and that the matrix A is *exactly* known. Often this assumption is not realistic because sampling or modeling or measurement errors also affect the matrix A. One way to take errors in A into account is to also introduce *perturbations in A* and consider the following TLS problem:

DEFINITION 2 (*The total least squares problem*). Given an overdetermined set of m linear equations $Ax \approx b$ in n unknowns x. The *total least squares problem is the following*:

$$\min_{[\hat{A};\hat{b}]\in\mathbb{R}^{m\times(n+1)}} \|[A;b]-[\hat{A};\hat{b}]\|_F \tag{12}$$

$$\text{subject to} \quad \hat{b}\in R(\hat{A})\,. \tag{13}$$

Once a minimizing $[\hat{A};\hat{b}]$ is found, then any x satisfying

$$\hat{A}x = \hat{b} \tag{14}$$

is called a *TLS solution* and $[\Delta\hat{A};\Delta\hat{b}] = [A;b] - [\hat{A};\hat{b}]$ the corresponding *TLS correction*.

The TLS solution is denoted by $\hat{x}$. It is clear that the TLS problem is a generalization of the LS problem as is formulated in Definition 1.

2. The basic algorithm

In this section, we will present the basic algorithm for solving the TLS problem. We will start with a brief review of the singular value decomposition (SVD) and some of its properties.

2.1. The singular value decomposition

The singular value decomposition (SVD) is of great theoretical and practical importance for the LS and TLS problems. Not only does it provide elegant geometrical and algebraic insights into many numerical linear algebra problems, but at the same time a numerically reliable algorithm can be devised [32].

THEOREM 1 (Singular value decomposition (SVD)). *If* $C\in\mathbb{R}^{m\times n}$ *then there exist orthonormal matrices* $U=[u_1,\ldots,u_m]\in\mathbb{R}^{m\times m}$ *and* $V=[v_1,\ldots,v_n]\in$

$\mathbb{R}^{n\times n}$ *such that*

$$U^{\mathrm{T}}CV = \Sigma = \operatorname{diag}(\sigma_1, \ldots, \sigma_p), \qquad \sigma_1 \geq \cdots \geq \sigma_p \geq 0 \text{ and}$$
$$p = \min\{m, n\}. \tag{15}$$

PROOF. For the proof, see [32, Theorem 2.5.1]. □

The σ_i are the *singular values* of C and they are collectively known as the *singular value spectrum*. The vectors u_i and v_i are the i-th *left singular vector* and the i-th *right singular vector*, respectively.

The SVD reveals many interesting structures of a matrix. If the SVD of C is given by Theorem 1, and we define r by

$$\sigma_1 \geq \cdots \geq \sigma_r > \sigma_{r+1} = \cdots = \sigma_p = 0,$$

the number of positive singular values, then

$$\operatorname{rank}(C) = r, \qquad R(C) = R([u_1, \ldots, u_r]) \text{ and}$$
$$N(C) = R([v_{r+1}, \ldots, v_n]).$$

Moreover, if $U_r = [u_1, \ldots, u_r]$, $\Sigma_r = \operatorname{diag}(\sigma_1, \ldots, \sigma_r)$, and $V_r = [v_1, \ldots, v_r]$, then we have the SVD expansion

$$C = U_r \Sigma_r V_r^{\mathrm{T}} = \sum_{i=1}^{r} \sigma_i u_i v_i^{\mathrm{T}}. \tag{16}$$

Equation (16) which is also called the *dyadic decomposition*, decomposes the matrix C of rank r in a sum of r rank one matrices.

From (15) it follows that

$$C^{\mathrm{T}}C = V\Sigma^{\mathrm{T}}\Sigma V^{\mathrm{T}} \quad \text{and} \quad CC^{\mathrm{T}} = U\Sigma\Sigma^{\mathrm{T}}U^{\mathrm{T}}.$$

Thus σ_i^2, $i = 1, \ldots, p$, are eigenvalues of the symmetric and nonnegative definite matrices $C^{\mathrm{T}}C$ and CC^{T}, and v_i and u_i are the corresponding eigenvectors. Hence, in principle, the SVD can be reduced to the eigenvalue problem for symmetric matrices. This is *not* a numerically suitable way to compute the SVD, as is shown in [12].

The SVD plays an important role in a number of matrix approximation problems. For our purpose the following is the most important, where we consider the approximation of one matrix by another of lower rank. Several other results and extensions can be found in [32, 80].

THEOREM 2 (Eckart–Young–Mirsky matrix approximation theorem). *Let the* SVD *of* $C \in \mathbb{R}^{m\times n}$ *be given by* $C = \sum_{i=1}^{r} \sigma_i u_i v_i^{\mathrm{T}}$ *with* $r = \operatorname{rank}(C)$. *If* $k < r$ *and* $C_k = \sum_{i=1}^{k} \sigma_i u_i v_i^{\mathrm{T}}$, *then*

$$\min_{\operatorname{rank}(D)=k} \|C - D\|_2 = \|C - C_k\|_2 = \sigma_{k+1} \tag{17}$$

and

$$\min_{\text{rank}(D)=k} \|C-D\|_F = \|C-C_k\|_F = \sqrt{\sum_{i=k+1}^{p} \sigma_i^2}\,, \quad p=\min\{m,n\}\,. \tag{18}$$

PROOF. For the proof, see [41, 21]. □

2.2. Basic solution

We now analyze the TLS problem by making substantial use of the SVD. As pointed out in [30] and more fully in [27, 31], this decomposition can be used to solve the TLS problem. Hereto we bring $Ax \approx b$ into the form

$$[A;b][x^T;-1]^T \approx 0\,. \tag{19}$$

Let the SVD of $[A;b]$ be

$$[A;b] = U\Sigma V^T = \sum_{i=0}^{n+1} \sigma_i u_i v_i^T\,, \quad \sigma_1 \geqslant \cdots \geqslant \sigma_{n+1} \geqslant 0\,. \tag{20}$$

If $\sigma_{n+1} \neq 0$, $[A;b]$ is of rank $n+1$ and the space S generated by the rows of $[A;b]$ coincides with $\mathbb{R}^{n+1}$. There is no nonzero vector in the orthogonal complement of S, hence the set of equations (19) is incompatible. In order to obtain a solution, the rank of $[A;b]$ must be reduced to n. Using the Eckart–Young–Mirsky theorem, the best rank n TLS approximation $[\hat{A};\hat{b}]$ of $[A;b]$, which minimizes the deviations in variance, is given by

$$[\hat{A};\hat{b}] = U\hat{\Sigma}V^T\,, \quad \text{with } \hat{\Sigma} = \text{diag}(\sigma_1, \ldots, \sigma_n, 0)\,.$$

The minimal TLS correction is then

$$\sigma_{n+1} = \min_{\text{rank}([\hat{A};\hat{b}])=n} \|[A;b]-[\hat{A};\hat{b}]\|_F$$

and is attained by

$$[A;b]-[\hat{A};\hat{b}] = [\Delta\hat{A};\Delta\hat{b}] = \sigma_{n+1}u_{n+1}v_{n+1}^T\,.$$

Note that this TLS correction matrix has rank one. It is clear that the approximate set

$$[\hat{A};\hat{b}][x^T;-1]^T = 0$$

is now compatible and its solution is given by the only vector v_{n+1} (i.e., the last column of V) which belongs to $N([\hat{A};\hat{b}])$. The TLS solution is then obtained by *scaling* v_{n+1} such that its last component is -1, i.e.,

$$[\hat{x}^T;-1]^T = \frac{-1}{v_{n+1,n+1}} v_{n+1}\,. \tag{21}$$

If $v_{n+1,n+1} \neq 0$, then $\hat{b} = \hat{A}\hat{x} \in R(\hat{A})$, i.e., equation (13) is satisfied, and hence $\hat{x}$ solves the basic TLS problem.

Observe that, if σ_{n+1} is zero, $[A; b]$ is of rank n and hence $v_{n+1} \in N([A; b])$. In this case, the set of equations (19) is compatible and no approximation is needed to obtain the exact solution, given by (21).

The following theorem gives conditions for the *uniqueness* and *existence* of a TLS solution.

THEOREM 3 (Solution of the basic TLS problem $Ax \approx b$). *Suppose* (20) *is the* SVD *of* $[A; b]$ *and* σ_n' *is the smallest singular value of* A. *If* $\sigma_n' > \sigma_{n+1}$, *then*

$$[\hat{A}; \hat{b}] = U\hat{\Sigma}V^{\mathrm{T}} \quad \textit{and} \quad \hat{\Sigma} = \operatorname{diag}(\sigma_1, \ldots, \sigma_n, 0) \tag{22}$$

with corresponding TLS *correction matrix*

$$[\Delta\hat{A}; \Delta\hat{b}] = [A; b] - [\hat{A}; \hat{b}] = \sigma_{n+1} u_{n+1} v_{n+1}^{\mathrm{T}} \tag{23}$$

solves the TLS *problem* (12)–(13) *and*

$$\hat{x} = -\frac{1}{v_{n+1,n+1}} [v_{1,n+1}, \ldots, v_{n,n+1}]^{\mathrm{T}} \tag{24}$$

exists and is the unique solution to $\hat{A}x = \hat{b}$.

PROOF. For the proof, see [72, Theorem 2.6]. □

It is interesting to note here that the conditions

$$\sigma_n' > \sigma_{n+1} \;\Leftrightarrow\; \sigma_n > \sigma_{n+1} \text{ and } v_{n+1,n+1} \neq 0$$

are equivalent, as is proven in [72, Corollary 3.4].

An illustration of the *geometry* of the TLS solution in the column space of A is depicted in Figure 2(b) for $n = 2$. The TLS problem is tantamount to finding a 'closest' subspace $R([\hat{A}; \hat{b}])$ to the $n + 1$ columns of $[A; b]$. Hereto, the sum of squared *perpendicular* distances from each column $a_i, b_i \in \mathbb{R}^m$ to $R([\hat{A}; \hat{b}])$ is minimized, and each column a_i, b_i is approximated by its orthogonal projection $\hat{a}_i, \hat{b}_i$ onto that subspace.

2.3. Basic algorithm

The following algorithm computes a TLS solution $\hat{x}$ of $Ax \approx b$ such that $(A - \Delta\hat{A})\hat{x} = b - \Delta\hat{b}$ and $\|[\Delta\hat{A}; \Delta\hat{b}]\|_{\mathrm{F}}$ is minimal.

ALGORITHM 1 (*Basic TLS solution of* $Ax \approx b$).
Given: $A \in \mathbb{R}^{m \times n}$ and $b \in \mathbb{R}^m$;
Step 1: Compute the SVD (20), i.e., $[A; b] = U\Sigma V^{\mathrm{T}}$;
Step 2: If $v_{n+1,n+1} \neq 0$ then $\hat{x} = -(1/v_{n+1,n+1})[v_{1,n+1}, \ldots, v_{n,n+1}]^{\mathrm{T}}$.
END

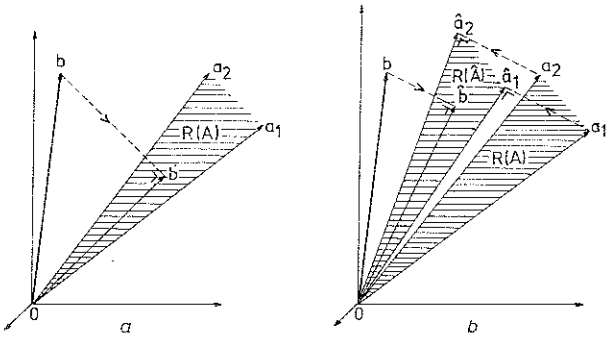


Fig. 2. (a) The LS solution is obtained by projecting b orthogonally onto $R(A)$ and solving $Ax = b'$. (b) The TLS solution is obtained by approximating the columns a_i of A and b by $\hat{a}_i$ and $\hat{b}$ until $\hat{b}$ is in the space $R(\hat{A})$, generated by the columns $\hat{a}_i$, and $\hat{A}x = \hat{b}$.

3. Extensions of the basic TLS algorithm

The basic algorithm discussed in the last section can only handle the case that $v_{n+1,n+1} \neq 0$. In this section, we will introduce the concept of nongeneric TLS solutions, and extend the results of the last section. Before we proceed, we first discuss the issue of nonuniqueness of the TLS solution in the generic case.

3.1. Nonuniqueness of the TLS solution

The condition $\sigma'_n > \sigma_{n+1}$, or equivalently, $\sigma_n > \sigma_{n+1}$ and $v_{n+1,n+1} \neq 0$, ensure that Algorithm 1 computes the *unique* TLS solution of $Ax \approx b$. These conditions are generically satisfied provided A is of full rank and the set $Ax \approx b$ is not highly noncompatible. Hence, most TLS problems which arise in practice can be solved by means of Algorithm 1.

Suppose now that $\sigma_n = \sigma_{n+1}$. Then the TLS problem (12)–(13) may still have a solution although it may not be unique. Indeed, any linear combination of the singular vectors $v_{p+1}, \ldots, v_{n+1}$ associated with the multiple singular value $\sigma_{p+1} = \cdots = \sigma_{n+1}$, $p < n$ and $\sigma_p > \sigma_{p+1}$, solves the TLS problem provided it results in a vector of the form $[\hat{x}^T; -1]^T$. The same conclusions apply to the case $m < n$, i.e., the set $Ax \approx b$ is *underdetermined*, since then the conditions $\sigma_{m+1} = \cdots = \sigma_{n+1} = 0$ hold. Whenever $\sigma_n = \sigma_{n+1}$, Algorithm 1 still computes a TLS solution which may be appropriate for the user. However, one often wants to single out the TLS solution with *minimal norm* $\|\hat{x}\|_2$ since this solution has minimal sensitivity. This suggests maximizing $v_{n+1,n+1}$ in Theorem 3 and can be accomplished as follows.

THEOREM 4 (Minimum norm TLS solution of $Ax \approx b$). *Consider the* TLS *problem* (12)–(14). *Let* (20) *be the* SVD *of* $[A; b]$ *and assume that* $\sigma_p > \sigma_{p+1} =$

$\cdots = \sigma_{n+1}$ *with* $p \leqslant n$. *Let* Q *be an orthonormal matrix such that*

$$[v_{p+1}, \ldots, v_{n+1}]Q = \begin{bmatrix} Y & z \\ 0 \cdots 0 & \gamma \end{bmatrix} \begin{matrix} n \\ 1 \end{matrix} \quad \begin{matrix} \\ \\ n-p & 1 \end{matrix}. \tag{25}$$

If $\gamma \neq 0$, *then the* TLS *solution*

$$\hat{x} = -z/\gamma \tag{26}$$

has minimal 2*-norm* $\|\hat{x}\|_2 = \sqrt{1-\gamma^2}/\gamma$.

The TLS *approximation and corresponding* TLS *correction matrix are given by*

$$[\hat{A}; \hat{b}] = [A - \Delta\hat{A}; b - \Delta\hat{b}] \quad \textit{with } [\Delta\hat{A}; \Delta\hat{b}] = [A; b]\begin{bmatrix} z \\ \gamma \end{bmatrix}[z^{\mathrm{T}}; \gamma]. \tag{27}$$

PROOF. For the proof, see [72, Theorem 3.7]. □

Closed-form expressions of the minimum norm TLS solution $\hat{x}$ are given in [72, Theorem 3.8].

In practice, singular values of $[A; b]$ will *rarely* coincide. Due to *errors* in the data, coinciding singular values of the corresponding unobservable exact relation $A_0 x_0 = b_0$ become *distinct*. In this case it is realistic to define an error bound ε such that all singular values σ_i, satisfying $|\sigma_i - \sigma_{n+1}| < \varepsilon$, are considered as coinciding with σ_{n+1} and the TLS solution is obtained as above (see also Section 3.3).

3.2. *Nongeneric TLS problems*

Whenever $v_{n+1,n+1} \neq 0$, the TLS problem (12)–(13) is *solvable* and is therefore called *generic*. The TLS solution can for instance be computed by Algorithm 1. Problems may occur whenever $v_{n+1,n+1} = 0$. In particular, if $\sigma_n > \sigma_{n+1}$ and $v_{n+1,n+1} = 0$, the TLS problem *fails* to have a solution altogether, as is shown below. More generally, if $\sigma_p > \sigma_{p+1} = \cdots = \sigma_{n+1}$, $p \leqslant n$, the TLS problem (12)–(13) fails to have a solution if all $v_{n+1,i} = 0$, $i = p+1, \ldots, n+1$. These problems are called *nongeneric* [66]. Let us consider an example [12].

EXAMPLE 1. (a) Let $n = 1$ and

$$[A; b] = \begin{bmatrix} 1 & 0 \\ 0 & 2 \end{bmatrix}.$$

Here $[A; b]$ is already in diagonal form and has a unique smallest singular value $\sigma_2 = 1$. Clearly, $v_2 = [1, 0]^{\mathrm{T}}$ and hence $v_{2,2} = 0$. The unique minimizing $[\Delta\hat{A}; \Delta\hat{b}]$ gives

$$[\hat{A}; \hat{b}] = [A - \Delta\hat{A}; b - \Delta\hat{b}] = \begin{bmatrix} 0 & 0 \\ 0 & 2 \end{bmatrix},$$

so the approximated set $\hat{A}x \approx \hat{b}$ is not compatible. However, an arbitrary small

perturbation ε in the $(2,1)$ entry will give a compatible set with solution $x = 2/\varepsilon$. Hence, there is no solution to the TLS problem (12)–(13).

(b) If $\operatorname{rank}(A) < n$ then the TLS problem has a solution only in the trivial case that $b \in R(A)$. Consider the example

$$A = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}, \qquad b = \begin{bmatrix} 1 \\ 1 \end{bmatrix}.$$

Here we have $b \in R(A - \Delta\hat{A})$ for $\Delta\hat{A} = \operatorname{diag}(0, \varepsilon)$ for any $\varepsilon \neq 0$, so there does not exist a smallest value of $\|[\Delta\hat{A}; \Delta\hat{b}]\|_F$. In the case when $\operatorname{rank}(A) < n$ we must add the constraint

$$\operatorname{rank}(A - \Delta\hat{A}) \leqslant \operatorname{rank}(A)$$

to the problem (12)–(13) in order to find a solution of the form $[\Delta\hat{A}; \Delta\hat{b}] = [A; b]vv^{\mathrm{T}}$.

Nongeneric TLS problems occur whenever A is rank-deficient ($\sigma_n' \approx 0$), or when the set of equations is highly noncompatible ($\sigma_n' \approx \sigma_{n+1}$ large). The latter situation is easily detected by inspecting the size of the smallest σ_i for which $v_{n+1,i} \neq 0$. If this singular value is large, the user can simply conclude that the data are not appropriate for linear modeling and as such reject the problem as irrelevant from a linear modeling point of view. In the first situation ($\sigma_n' \approx 0$), two options are possible. First, the user can remove the dependency between the columns of A by removing appropriate columns in A such that the remaining submatrix A_p of dimension $m \times p$, $p < n$, has full rank and then apply TLS to the reduced problem $A_p x \approx b$ in order to obtain an estimate of the remaining parameters. The position of the nonzero entries in v_{n+1} determines which columns of A, i.e., which variables in the model, are dependent. How to pick these columns is a problem of *subset selection*. Procedures for discarding or selecting columns in A are available in a variety of settings, e.g., see [33, 34, 64, 32, Section 12.2]. Another way is to solve a nongeneric TLS problem, i.e., additional constraints are imposed on the TLS problem (12)–(13) in order to make the problem solvable.

The properties of these problems are described in [72, Theorem 3.11]. In particular, let

$$A = U'\Sigma'V'^{\mathrm{T}} = \sum_{i=1}^{n} \sigma_i' u_i' v_i'^{\mathrm{T}}, \quad \sigma_1' \geqslant \cdots \geqslant \sigma_n' \geqslant 0 \tag{28}$$

be the SVD of A and (20) be the SVD of $[A; b]$. Let b' be the orthogonal projection of b onto $R(A)$ and $[\hat{A}; \hat{b}]$ be given by (22). If $\sigma_n > \sigma_{n+1}$ and $v_{n+1,n+1} = 0$, then this theorem proves that

$$\sigma_{n+1} = \sigma_n', \qquad u_{n+1} = \pm u_n', \qquad v_{n+1} = \begin{bmatrix} \pm v_n' \\ 0 \end{bmatrix} \tag{29}$$

and b, b' as well as $\hat{b}$ are orthogonal to u_n'.

It is easy to see that the generic TLS approximation $[\hat{A}; \hat{b}]$ and corresponding

TLS correction matrix $[\Delta\hat{A}; \Delta\hat{b}]$ (see Theorem 3) minimizes $\|[\Delta\hat{A}; \Delta\hat{b}]\|_F$ but does *not* satisfy the constraint $\hat{b} \in R(\hat{A})$ and therefore, this $[\hat{A}; \hat{b}]$ does not solve the TLS problem (12)–(13). Indeed, using (28), (20) and (29), one obtains

$$[\hat{A}; \hat{b}] = [A; b] - [\Delta\hat{A}; \Delta\hat{b}] = [A; b] - \sigma_{n+1} u_{n+1} v_{n+1}^T$$
$$= \left[\sum_{i=1}^{n} \sigma_i' u_i' v_i'^T; b\right] - \sigma_n' u_n' [v_n'^T; 0] = \left[\sum_{i=1}^{n-1} \sigma_i' u_i' v_i'^T; b\right].$$

Observe that this approximation makes $\hat{A}$ rank-deficient! Indeed, A is reduced to a matrix $\hat{A}$ of rank $n-1$ while b is not changed at all. Since $\operatorname{rank}(\hat{A}) = n - 1 < \operatorname{rank}([\hat{A}; \hat{b}]) = n$, it follows that $\hat{b} \notin R(\hat{A})$. Moreover, (29) also yields

$$[\hat{A}; \hat{b}] v_{n+1} = 0 \Rightarrow \hat{A} v_n' = 0,$$
$$[A; b] v_{n+1} = \sigma_{n+1} u_{n+1} \Rightarrow A v_n' + 0 \cdot b = A v_n' = \sigma_n' u_n' \approx 0 \quad \text{if } \sigma_n' \approx 0. \tag{30}$$

This means that the solution v_n' of the set $\hat{A}x = 0$ describes an approximate linear relation among the columns of A instead of estimating the desired linear relation between A and b.

In these situations, the generic TLS problem (12)–(13) as such has no meaningful solution, as is shown in the examples above. Moreover, this approach makes the problem *very ill-conditioned*. Indeed, since ε must be as small as possible, the coefficients of the generic TLS solution $\hat{x}$ are inflated and have *large* variances. Therefore, we propose here a *nongeneric* solution which still satisfies the TLS criteria (12)–(13) under the *additional constraint* that $[\Delta\hat{A}; \Delta\hat{b}]\, v_{n+1} = 0$ or equivalently $\begin{bmatrix} \hat{x} \\ -1 \end{bmatrix} \perp v_{n+1}$.

DEFINITION 3 (*The nongeneric one-dimensional total least squares problem*). Given an overdetermined set of m linear equations $Ax \approx b$ in n unknowns x. Let (20) be the SVD of $[A; b]$. The *nongeneric one-dimensional total least squares (TLS) problem* is

$$\min_{[\hat{A}; \hat{b}] \in \mathbb{R}^{m \times (n+1)}} \|[A; b] - [\hat{A}; \hat{b}]\|_F \tag{31}$$

$$\text{subject to} \quad \hat{b} \in R(\hat{A}), \tag{32}$$

$$[\Delta\hat{A}; \Delta\hat{b}] v_j = 0 \quad \forall j: \max_{v_{n+1,p} \neq 0} \{p\} < j \leq n+1. \tag{33}$$

Once a minimizing $[\hat{A}; \hat{b}]$ is found, then any x satisfying

$$\hat{A}x = \hat{b} \tag{34}$$

is called a *nongeneric TLS solution*, and $[\Delta\hat{A}; \Delta\hat{b}] = [A; b] - [\hat{A}; \hat{b}]$ the corresponding *nongeneric TLS correction*.

Since (33)$\Leftrightarrow \begin{bmatrix} x \\ -1 \end{bmatrix} \perp v_j$, $j = p+1, \ldots, n+1$ (provided $v_{n+1,p} \neq 0$), one could as well use the latter constraints instead of (33).

The introduction of the *additional constraints* $\begin{bmatrix} x \\ -1 \end{bmatrix} \perp v_j$, $\forall j$ with $v_{n+1,j} = 0$ in the nongeneric TLS approach can be motivated as follows. The singular vectors v_j with negligible or zero last component and associated with a small singular value, are called *nonpredictive multicollinearities* in linear regression since they reveal multicollinearities (i.e., approximate linear dependencies between the columns of A) in A that are of no (or negligible) value in predicting the response b. In fact if $v_{n+1,n+1} = 0$, then using (29) yields (30). Since $\sigma'_n = \sigma_{n+1}$ is the smallest singular value, this means that A is nearly rank-deficient or else the set of equations is highly noncompatible. Since also $b \perp u'_n = u_{n+1}$, according to (29), there is *no correlation* between A and b in the direction of $u'_n = u_{n+1}$. Hence, it does not make sense here to induce a correlation between $\hat{A}$ and $\hat{b}$ in the direction u_{n+1}. This would induce a wrong interpretation about the exact relation between A and b. If $b \perp u_{n+1}$ then keep also the TLS approximation $\hat{b} \perp u_{n+1}$ as done in our nongeneric TLS approach. Therefore, the strategy of nongeneric TLS is to eliminate those directions in A which are *not* at all correlated with the observation vector b. Indeed, solving a set of equations is computing the relation between A and b. If there is no correlation between b and a left singular vector u'_j of A, i.e., $b \perp u'_j$, it is better to eliminate that direction rather than forcing a solution in that direction.

Latent root regression [76] follows a similar approach. It minimizes the residual sum of squares $\|Ax - b\|_2^2$ subject to the *same* constraints, i.e., $\begin{bmatrix} x \\ -1 \end{bmatrix} \perp \{\text{all nonpredictive } v_j\}$. Hence, if there are no nonpredictive v_j, then the latent root regression estimate equals the LS solution. This is a way of *stabilizing* the solution in linear regression when the data in A are nearly multicollinear ($\sigma'_n \approx 0$). It is well known that then the ordinary LS solution tends to be inflated and predicted values may be unreasonable.

The nongeneric TLS solution is another way of handling this multicollinearity problem and stabilizing the TLS solution. Nongeneric TLS minimizes the applied corrections $\|[A - \hat{A}; b - \hat{b}]\|_F$ subject to $\hat{A}x = \hat{b}$ and the *same* constraints as used in latent root regression. If there are *no* nonpredictive v_j, then the nongeneric TLS solution equals the generic TLS solution. This is proven in our next theorem.

THEOREM 5 (Nongeneric one-dimensional TLS solution). *Let* (20) *be the* SVD *of* $[A; b]$ *and assume* $v_{n+1,j} = 0$ *for* $j = p+1, \ldots, n+1$, $p \leq n$. *If* $\sigma_{p-1} > \sigma_p$ *and* $v_{n+1,p} \neq 0$, *then*

$$[\hat{A}; \hat{b}] = U\hat{\Sigma}V^T \quad \textit{with } \hat{\Sigma} = \operatorname{diag}(\sigma_1, \ldots, \sigma_{p-1}, 0, \sigma_{p+1}, \ldots, \sigma_{n+1}) \tag{35}$$

with corresponding nongeneric TLS *correction matrix*

$$[\Delta\hat{A}; \Delta\hat{b}] = [A; b] - [\hat{A}; \hat{b}] = \sigma_p u_p v_p^T \tag{36}$$

solves the nongeneric TLS *problem* (31)–(33) *and*

$$\hat{x} = -\frac{1}{v_{n+1,p}}[v_{1,p}, \ldots, v_{n,p}]^T \tag{37}$$

exists and is the unique solution to $\hat{A}x = \hat{b}$.

PROOF. For the proof, see [72, Theorem 3.12]. □

In numerical practice, $v_{n+1,j}$ will seldom be zero. Indeed, due to errors in the observations $[A; b]$, a zero-valued $v_{n+1,j}$ in the SVD of the unobservable true data matrix $[A_0; b_0]$ will differ from zero in the SVD of $[A; b]$. Hence, it is advisable to define an error bound ε such that all $|v_{n+1,j}| < \varepsilon$ are considered to be zero (see Section 3.3).

It should be noted that nongeneric TLS problems do not occur if one is only interested in estimating a linear relationship between the columns of $[A; b]$, no matter which column is used as right-hand side. If then $v_{n+1,n+1} = 0$, one simply replaces b by any column a_i of A provided $v_{i,n+1} \neq 0$.

3.3. *Extended TLS algorithm*

We now summarize the practical TLS computations into one algorithm which solves any generic and nongeneric TLS problem with one right-hand side. In case of nonuniqueness, the minimum norm TLS solution is computed. A fully documented Fortran 77 program of this classical TLS algorithm is given in [61, 59]. The code can be obtained through netlib [20].

ALGORITHM 2 (*(Non)generic TLS solution* $\hat{x}$ *of* $Ax \approx b$).

Given: An $m \times n$ data matrix A and an $m \times 1$ observation vector b.

Step 1: *SVD of* $[A; b]$. Compute the singular value decomposition (20) of $[A; b]$.

Step 2: *Rank determination*. If not user determined, compute the numerical rank r $(\leq n)$ of $[A; b]$ as follows

$$\sigma_1 \geqslant \cdots \geqslant \sigma_r > R_\nu \geqslant \sigma_{r+1} \geqslant \cdots \geqslant \sigma_{n+1} \tag{38}$$

with R_ν an appropriate rank determinator.

Step 3: *TLS solution* $\hat{x}$. Compute with Householder transformations the orthogonal matrix Q such that

$$[v_{r+1}, \ldots, v_{n+1}]Q = \begin{bmatrix} Y & z \\ 0 & \gamma \end{bmatrix} \begin{matrix} n \\ 1 \end{matrix} \tag{39}$$
$$\qquad\qquad\quad n-r \quad 1$$

If $|\gamma| < \varepsilon$ then

begin {*TLS solution is nongeneric*}
lower the rank r with the multiplicity of σ_r
go back to the beginning of Step 3
end
else $\hat{x} = -(1/v_{n+1,n+1})[v_{1,n+1}, \ldots, v_{n,n+1}]^T$.

END

4. More efficient TLS algorithms

In this section, we will present some methods that will enhance the efficiency of the algorithms discussed before. We will also discuss some iterative methods that are more suitable for large sparse problems.

4.1. Direct speed improvement

Observe from (39) that we only need to compute a *few* singular vectors, associated with the smallest singular values of $[A; b]$ in order to obtain the TLS solution $\hat{x}$. Moreover, we only need to compute a *basis* of the singular subspace corresponding to the smallest $n + 1 - r$ singular values with r the numerical rank of $[A; b]$. Based on these properties Van Huffel and Vandewalle [65] were able to *improve the efficiency* of the TLS computations by computing the SVD of $[A; b]$ in Step 1 only '*partially*'. This results in the development of an *improved algorithm PSVD* which computes the singular subspace of a matrix, associated with its smallest singular values. There are three reasons for its high efficiency with respect to the classical SVD algorithm. First, the Householder transformations of the bidiagonalization are only applied to the basis vectors of the desired singular subspace. Second, the bidiagonal matrix is only partially diagonalized and third, an appropriate choice is made between QR and QL iteration steps. Incorporating the 'partial SVD' algorithm into the TLS computations, results in an *improved 'partial TLS' algorithm PTLS*. Its higher efficiency with respect to the classical TLS algorithm is demonstrated and confirmed with computational results (see [72, Section 4.5; 65]). Typically, PTLS reduces the computation time with a factor 2.

An alternative method for computing the basis of a left and/or right singular subspace of a matrix associated with its smallest singular values, appeared recently [15, 16]. Similarly to PSVD, this method does not need to compute the complete SVD but instead uses a *rank revealing QR factorization* (RRQR), i.e., a QR factorization of a matrix C in the particular form

$$C_{m\times n}\Pi = QR = Q\begin{bmatrix} R_{11} & R_{12} \\ 0 & R_{22} \end{bmatrix}\begin{matrix} r \\ n-r \end{matrix} \quad \text{with } r \text{ the numerical rank of } C \tag{40}$$

and $\|R_{22}\|_2$ small such that any numerical rank deficiency in C is revealed. Chan [14] has described an algorithm for choosing the permutation Π that

guarantees $\|R_{22}\|_2$ to be small. Using this RRQR, upper and lower bounds for the small singular values are easily obtained and used to compute the numerical rank r of C. The RRQR also yields approximations to the corresponding $n-r$ singular vectors, which are then further improved by means of inverse subspace iteration. Finally, these vectors can be used to compute the TLS solution $\hat{x}$ of $Ax \approx b$, $C=[A;b]$, by performing Step 3 of Algorithm 2. As long as the matrix C has a well-determined numerical rank r, i.e., the gap between σ_r and σ_{r+1} is large, and the nullity is small compared to the dimensions of the matrix, the computational complexity of the RRQR algorithm is only slightly larger than that of the ordinary QR algorithm. Moreover, Bischof and Hansen [11] have recently demonstrated how the RRQR factorization of a sparse matrix can be computed efficiently without destroying the sparsity pattern of the matrix. Since PSVD carries out a complete reduction to bidiagonal form, it is not well suited for general sparse matrices. Based on this analysis, Chan and Hansen concluded that the RRQR based TLS algorithm described in [15, 16] is actually less demanding than PTLS, mainly because a reduction to bidiagonal form is avoided. It should be noted that their conclusions primarily hold when the nullity $n-r$, i.e., the dimension of the numerical null space of $[A;b]_{m\times n}$, is small, the gap between σ_r and σ_{r+1} is large and the TLS problem is not close-to-nongeneric. However, when the gap is not so large, the RRQR based TLS algorithm is still able to give good results but at the cost of a larger computational effort involved in the large number of inverse subspace iterations.

Finally, we mention that, based on the concept of the RRQR factorization, Stewart [56] recently proposed the so-called *rank revealing URV* decomposition. Let $C_{m\times n}$ be of numerical rank r such that its singular values satisfy $\sigma_1 \geqslant \cdots \geqslant \sigma_r > \sigma_{r+1} \geqslant \cdots \geqslant \sigma_n$ where σ_r is large compared to σ_{r+1}. Then, C can be decomposed into the form

$$C = U\begin{bmatrix} R & F \\ 0 & G \end{bmatrix}V^{\mathrm{T}},$$

where U, V are orthogonal, R and G are upper triangular, σ_r approaches the minimal singular value of R and $\|F\|_{\mathrm{F}}^2 + \|G\|_{\mathrm{F}}^2 \approx \sigma_{r+1}^2 + \cdots + \sigma_n^2$. It is shown that this decomposition is equally effective as the SVD in exhibiting the null space. In contrast to the RRQR, this decomposition exhibits the null space of C explicitly. Moreover, it is shown that this decomposition is equally effective as the SVD in exhibiting the null space of a matrix but is computationally much more efficient and can be easily updated in an efficient way. Replacing the classical SVD in the TLS algorithm by a RR URV decomposition leads to an efficient and reliable TLS algorithm that can be parallelized in an efficient way [74].

4.2. Iterative speed improvement

If *a priori information* is available, the computation time can be further reduced by using an *iterative* algorithm. This happens for instance in the

estimation of parameters of nonstationary systems that slowly vary with time, space or frequency. In these problems, slowly varying systems of equations have to be solved at each time instant and the TLS solution at step t is usually a good initial guess for the solution at step $t+1$. Therefore, *iterative algorithms* are more efficient since these methods include this a priori information in the choice of their starting vector or matrix. Two types of *varying* data sequences are possible. The changes in the data matrix at each step can be of rank *one* (or two), e.g., when a new column or row is added or deleted. In these cases, the computation time can be sped up considerably by using efficient rank 1 updating algorithms [32, Section 12.6]. In other situations, e.g., block-processing, the changes are of small norm but still of *full* rank, e.g., when all elements of the data matrix change slowly from step to step.

There are still other reasons for preferring iterative methods in high speed computing. Each step of an iteration routine gives a new and better estimate of the solution. This allows to control the level of convergence depending on the perturbations of the data. Furthermore, iterative algorithms are easy to code. Finally, an iterative algorithm enables us to use the given matrix over and over again without modifying it during the computation. This is most important if the matrix itself is highly structured or sparse.

In [72, Chapter 5; 62] various iterative algorithms are compared for solving slowly varying TLS problems $Ax \approx b$ of small or *moderate* size that require at each time instant the computation of the singular subspace of the data matrix $[A; b]$ associated with its smallest singular values. In particular, inverse iteration, ordinary Chebyshev iteration and inverse Chebyshev iteration are discussed. Also, Rayleigh quotient iteration and the Lanczos methods are briefly described. By analyzing the convergence properties of these methods, it is shown that inverse iteration is generally the *best* choice in terms of efficiency and ease-of-use provided the ratio between the singular values, corresponding to the desired and undesired singular subspace of the matrix $C = [A; b]$, is high. If this ratio is small, say less than one order of magnitude, convergence can be *accelerated* by applying the Chebyshev polynomials instead of the inverse power functions to the cross-product matrix $C^T C$ (resp., $(C^T C)^{-1}$). This method is called *ordinary* (resp., *inverse*) Chebyshev iteration. Inverse Chebyshev iteration is proven to converge always *faster*, mostly considerably, to the desired basis than ordinary Chebyshev iteration. Moreover, this method converges always *faster* than inverse iteration provided a lower bound sufficiently close to the undesired squared singular value spectrum is known. The smaller the gap, the larger the gain in speed. Ordinary Chebyshev iteration is only efficient in problems characterized by a very dense singular value spectrum. The (inverse) Lanczos method is shown to have a similar convergence behavior as (inverse) Chebyshev iteration with optimal bounds. Moreover, no bounds on the singular values need be known. Note however that roundoff errors make the Lanczos methods difficult to use in practice. Additional computations are required which reduce their computational efficiency and question their practical use in moderately sized TLS problems.

Based on the convergence rate and the number of operations in each iteration step, the efficiency of iterative methods can be compared with that of the direct computation methods: classical and partial SVD. It is concluded that iterative methods are most efficient when only *one* singular vector is to be computed, their convergence rate is sufficiently *high*, the desired accuracy is rather low and a good start vector is available. Iterative methods are therefore particularly attractive in solving slowly varying TLS problems because then the solution of a previous set is mostly a good initial guess for the solution of the next set.

5. TLS applications

The improved results obtained so far in TLS applications enhance the widespread use of this method. There are basically three situations in which TLS is most useful.

First of all, TLS has been proven useful in models with *only measurement error*. These models, referred to as classical *errors-in-variables* (EIV) models, are characterized by the fact that the true values of the observed variables satisfy one or more unknown but exact linear relations of the form (1). If the errors in the observations are independent random variables with zero mean and equal variance, TLS gives better estimates than LS does, as confirmed by simulations [69, 67, 72, 7, 6]. This situation may occur far more often in practice than is recognized. It is very common in agricultural, medical and economic sciences, in humanities, business and many other data analysis situations. Hence TLS should prove to be a quite useful tool to data analysts. An important caveat should be noted. The EIV model is useful when the primary goal is model parameter estimation rather than prediction. If one wishes to predict new values b_i^0 of β given additional measurements a_i of α in model (3)–(4), ordinary LS should normally be used. Also, if the data significantly violate the model assumptions, e.g., when outliers are present, the accuracy of the TLS estimates deteriorates considerably [7, 6]. Also LS encounters stability problems, although less dramatically. In these situations, *robust* procedures which are quite efficient and rather insensitive to outliers, should be applied, e.g., [17, 79].

A second application of TLS stems from the immediate connection between TLS and *orthogonal least squares fitting*. TLS fits a linear manifold of dimension s, $1 \leqslant s \leqslant n$, to a given set of points in $\mathbb{R}^{n+1}$ (the rows of $[A; b]$ in (2)) such that the sum of orthogonal squared distances from these points to the manifold attains a minimum [52].

Third, TLS is particularly useful in modeling situations in which the variables α_i and β in (1) should be treated *symmetrically*. These situations frequently occur in scientific and technical measurement when one is interested in the parameters of a model only and not in predicting one variable from other variables. For example, in models with only measurement error, the variables

enter the model in a symmetric manner from a distributional point of view but we generally choose to identify one variable as the β variable.

We now point out in different fields more specific TLS applications in order to illustrate the improvements obtained so far by using the TLS. This set of examples is certainly not exhaustive and is only intended to give the reader some sense of the diversity of the applications of the method.

First of all, the use of TLS for handling *multicollinearities*, i.e., nearly exact linear relations among the independent variables α_i of model (1), is discussed. In multivariate regression, linear or nonlinear, multicollinearities among the independent variables sometimes cause severe problems. The estimated coefficients can be very unstable and therefore far from their real values. In particular, this makes predictions by the regression model inaccurate. In many chemical applications of multivariate regression, like the example presented in [77] of relationships between chemical structure and biological activity, the predictive properties of the model are of prime importance and the regression estimates therefore often need to be stabilized. The example in [77] shows that the minimum norm TLS solution to the multivariate regression problem is stabilized, as opposed to the LS solution, and has (at least in the example investigated) minimal prediction error compared to all other biased regression

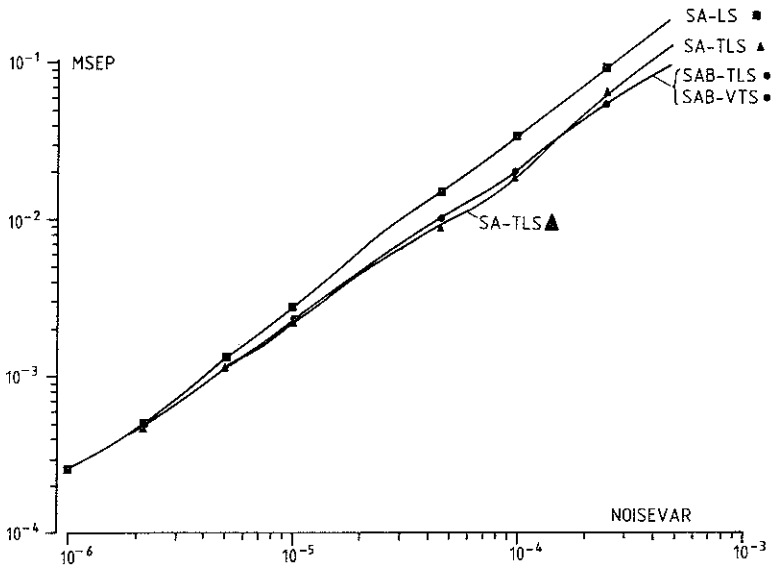


Fig. 3. Comparison of SA-LS, SA-TLS, SAB-TLS, and SAB-VTS: mean squared error of prediction (MSEP), computed over 100 noisy sets of equations, versus the variance of the noise added to the exact original model $(A_0)_{30\times 10}x = b_0$. The singular values of A_0 are 10, 5, 1, 0.5, 0.1, 0, 0, 0, 0, 0. Hence, 5 variables must be deleted. $b_0 = \Sigma_{i=1}^{5}(1/\sqrt{5})u_i$, where u_i is the i-th left singular vector of A_0.

estimators studied here. Stabilization is performed by reducing the matrix of observations $[A; b]$ to a matrix of smaller rank.

In applications, the multicollinearity problem is often handled by selecting a subset of variables such that the size of the subset equals the estimated rank r of the matrix $[A; b]$. How to choose these r variables α_i which are to be used in approximating the response β in (1), is the problem of *subset selection*. If now all variables are observed with zero-mean random errors of equal variance, the TLS method can be successfully applied. A subset selection algorithm SAB-TLS, based on TLS, has been developed [64, 60]. Its selection properties and accuracy in parameter estimation and prediction have been evaluated with respect to the subset selection algorithm SA-LS of Golub, Klema and Stewart [32, Section 12.2]. Only the need of predicting future responses β in the true system is considered here, e.g., in hypotheses and simulation studies. The TLS concept typically applies to those cases. The SA-LS algorithm is recommended if the variables in the data matrix A are assumed to be free of error. As soon as the variables are unobservable and only perturbed data are available, the TLS technique should be used in order to obtain the most accurate estimates for the parameters in any selected subset model. This is shown in Figure 3. If the perturbations are sufficiently small, subset selection based on the r-th right singular subspace of A (SA-TLS) enables a slightly better prediction accuracy in the case of bad subset condition. In all other cases, namely in case of well-conditioned or highly perturbed data sets, subset selection based on the r-th right singular subspace of $[A; b]$ (SAB-TLS) yields a better *prediction accuracy*. By taking into account the extra information provided by the observation vector b, SAB-TLS computes the best subset and attains a better and longer stability in its subset choice. A computationally attractive variant SAB-VTS of the subset selection algorithm SAB-TLS, which enables the same prediction accuracy (see Figure 3), was also derived.

In the following we explore the use of TLS in the field of *time domain system identification* and *parameter estimation*. A wide variety of different models are used to describe the system behavior in the time domain. If the process can be modeled as a linear, time-invariant, causal, finite-dimensional system with zero-initial state, then an *impulse response model* may be used

$$y(t) = \sum_{k=0}^{n} h(k)u(t-k)\,, \tag{41}$$

$h(k)$ is the impulse response of the system at time instant k. The system is identified if its impulse response can be estimated from observations of the inputs $u(t)$ and outputs $y(t)$ over a certain interval of time $t = -n, \ldots, m$. This so-called *deconvolution* problem is essentially reduced to a problem of solving a set of linear equations by writing (41) for $t = 0, \ldots, m$,

$$Y = UH\,,$$

i.e.,

$$\begin{bmatrix} y(0) \\ \vdots \\ y(m) \end{bmatrix} = \begin{bmatrix} u(0) & u(-1) & \cdots & u(-n) \\ u(1) & u(0) & \cdots & u(1-n) \\ \vdots & \vdots & \ddots & \vdots \\ u(m) & u(m-1) & \cdots & u(m-n) \end{bmatrix} \begin{bmatrix} h(0) \\ \vdots \\ h(n) \end{bmatrix}. \tag{42}$$

U is the data matrix obtained from (41) and H contains the unknown model parameters $h(k)$. By taking more data samples such that $m > n$, the accuracy can be improved. Assume now that all observed inputs and outputs are perturbed by independent, time-invariant, zero-mean white noise processes of equal variance, then one obtains a more accurate impulse response by solving (42) with TLS instead of LS, as confirmed by simulations [60, 63]. Taking account of the Toeplitz structure of the data matrix U further improves the accuracy but these so-called 'constrained' TLS problems are hard to solve [1–4].

The TLS method has been applied as a deconvolution technique in a practical real-life problem, encountered in *renography* [71]. An intravenous injection of a radioactive tracer that is cleared by the kidneys is administered, and the radioactivity over each kidney, as well as over the renal artery, is measured during a certain time period and visualized in a diagram (see Figure 4). Using these samples, the desired renal retention function, which yields useful clinical data, is obtained by deconvolution. Results from simulations, as well as from clinical data, show the advantages of the TLS technique with respect to the matrix algorithm [36, 58]. This last method is the most current deconvolution technique for calculating the renal retention function from (42) and is based on back-substitution or Gaussian elimination. As is well known in linear algebra, this method is very sensitive to errors on the data. To counteract this problem, the original curves are then usually smoothed.

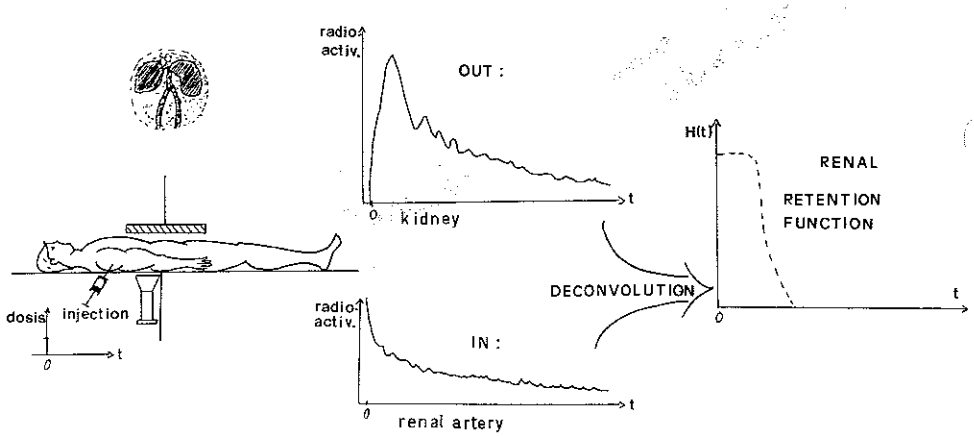


Fig. 4. After the injection of a radioactive tracer into an antecubital vein of the patient, the radioactive counts in each kidney, as well as in the renal artery, are enregistered during a certain time interval (20–30 min) and visualized in an activity–time curve. Using these samples, the desired renal retention function is computed by deconvolution.

It is concluded that the TLS method is more accurate, more powerful and more reliable than the matrix algorithm (MA), even if the curves are smoothed. As shown in Figure 5, the accuracy of MA depends strongly on the number of smoothings carried out on the curves. Using TLS, the curves need not be smoothed. Indeed, smoothing does not improve the accuracy of the retention function computed with TLS. Moreover, MA can only solve full rank problems. This implies that the method fails to compute the retention function when the data result in a (nearly) rank-deficient set (42) of convolution equations. TLS however can easily reduce the rank of the matrix involved and still compute a reliable retention function.

Another frequently used model to describe a system behavior in the time domain is the *transfer function* model which essentially expresses an *autoregressive moving average* (ARMA) relation between the inputs $\{u(t)\}$ and the outputs $\{y(t)\}$ fed to the system,

$$y(t) + a_1 y(t-1) + \cdots + a_{n_a} y(t-n_a) = b_1 u(t-1) + \cdots + b_{n_b} u(t-n_b)\,. \tag{43}$$

$\{a_j\}$ and $\{b_j\}$ are the unknown constant parameters of the system. If sufficient observations are taken, (43) gives rise to an overdetermined Toeplitz-like set of equations. If the observed inputs and outputs are perturbed by mutually

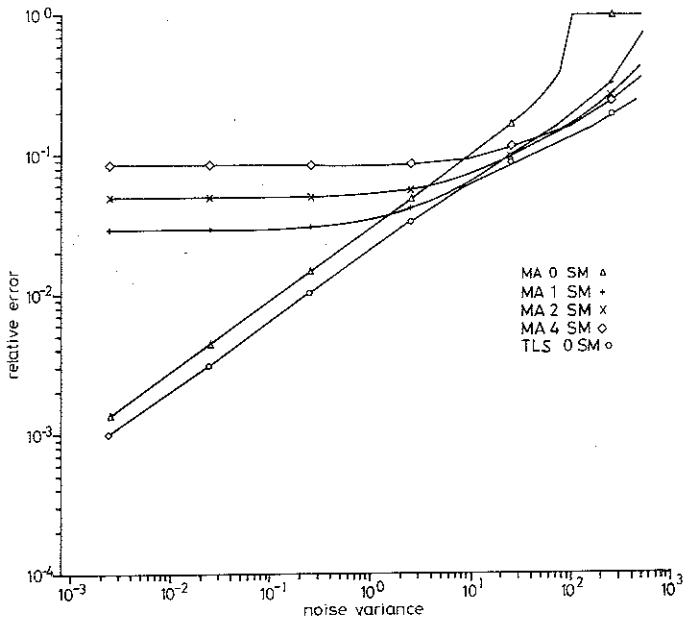


Fig. 5. Comparison of the accuracy of the impulse response computed by MA with smoothing and TLS without smoothing: a log–log diagram shows the average relative error (over 100 noisy sets) versus the variance of the noise added to an exact set of convolution equations, derived from the ideal curves. Errors larger than one are set equal to one. 0, 1, 2 and 4 correspond with the number of smoothings carried out on the curves.

independent time-invariant zero-mean white noise sequences of equal variance, the TLS solution of this set, coinciding with the Koopmans–Levin estimate [22], can be computed here. Necessary and sufficient conditions for consistency, similar to those given for EIV models [26, 25, 24, 49], have been derived [9, 68]. Although the TLS method is asymptotically not necessary more accurate than the ordinary instrumental variable (IV) method with delayed inputs as instruments [57], Van Huffel and Vandewalle [70] proved by means of simulations that TLS outperforms the IV methods in models of the form (43) when *short* sample lengths are used. Mostly, the TLS method is superior in terms of both bias and variance and gives estimates with smaller mean squared error (MSE) than the ordinary IV methods. The MSE becomes comparable by extending the IV sufficiently. The better accuracy of TLS is particularly clear in cases where the zeros of the polynomial $1 + a_1 z + \cdots + a_{n_a} z^{n_a}$ are *close* to the unit circle or where *both* the inputs and outputs are noisy. In other cases, TLS and IV methods give quite similar results.

Other applications in the field of system identification to which TLS has been successfully applied are surveyed in [72, Chapter 1].

Also in the field of modern *signal processing* the TLS approach is under study and is proved to be useful, e.g., in estimating the *frequencies* and *amplitudes* or powers of multiple *complex sinusoids in white noise*. This problem arises in numerous applications encountered in such diverse fields as radar, sonar, exploration seismology and radio astronomy. A variety of algorithms for this so-called *harmonic retrieval* problem [44] has been proposed and analyzed over the past few decades. We only cite here the TLS based contributions (although not always explicitly stated), such as the algebraic approach of Pisarenko [44], the linear prediction based work of Rahman and Yu [45], the rotational invariance technique ESPRIT of Roy and Kailath [47, 48], as well as the Procrustes rotations based ESPRIT algorithm proposed recently by Zoltowski and Stavrinides [83]. The latter two algorithms have also been applied to the more general class of practical signal processing problems whose objective is to estimate from measurements a set of constant parameters upon which the received signals depend, e.g., in high resolution *direction-of-arrival* (DOA) estimation.

Furthermore, TLS has been successfully applied in the field of experimental modal analysis [38], in acoustic radiation, geology, inverse scattering, Hamiltonian systems, etc. (see [72] for a list of references).

Finally, we mention that the TLS concept has been applied to *nonlinear* models in which the true variables are nonlinearly related to each other. The independent variables, as well as the observations, may have errors. Golub and LeVeque [29] presented two algorithms for solving separable nonlinear TLS problems. Other algorithms are discussed in [13, 50, 51].

This list of TLS applications is certainly not exhaustive. Currently, the use of TLS in geophysical tomographic imaging and oceanographic data analysis, in three-dimensional motion registration and in parameter estimation for partial differential equations, as well as in nonlinear regression, is being investigated.

However, there still remain a lot of *unexplored* problems where TLS could be successfully applied to improve the quality of the results.

6. Concluding remarks and generalizations

Solving sets of linear equations is a basic issue in many applications. If these sets $Ax \approx b$ are overdetermined, then generally only an approximate solution can be computed, for instance by using a LS or TLS approach.

The basic principle of TLS is that the noisy data $[A; b]$, while not satisfying a linear relation, are modified with minimal effort, as measured by the Frobenius norm, in a 'nearby' matrix $[\hat{A}; \hat{b}]$ which is rank-deficient so that the set $\hat{A}x = \hat{b}$ is compatible. This matrix $[\hat{A}; \hat{b}]$ is a rank one modification of the data matrix $[A; b]$. The solution to the TLS problem can be determined from the SVD of the matrix $[A; b]$. A simple algorithm outlines the computations of the solution of the basic TLS problem. By 'basic' is meant that only one right-hand side vector b is considered (one-dimensional) and that the TLS problem is solvable (generic) and has a unique solution. Extensions of this basic TLS problem are investigated in Section 3 and the TLS computations are summarized in one algorithm.

Since the TLS solution is deduced from only one right singular vector or in general, a basis of the right singular subspace associated with the smallest singular values of $[A; b]$, more efficient algorithms can be developed which only calculate those desired basis vectors, as surveyed in Section 4. The TLS approach has been proven useful in a lot of applications, as surveyed in Section 5.

So far only TLS problems $Ax \approx b$ with *one* right-hand side vector b are considered here. These problems are called *one-dimensional* in contrast to multidimensional problems $AX \approx B_{m \times d}$ characterized by d (>1) right-hand side vectors. The latter problems can be solved by computing the TLS solution of each subproblem $Ax_i \approx b_i$, $i = 1, \ldots, d$ separately. Hereto, Algorithm 1 or ` can be used. A better way of computation, at least when all data are equally perturbed and all subproblems $Ax_i \approx b_i$ have the same degree of noncompatibility, is to solve the multidimensional TLS problem $AX \approx B$. These problems are studied in detail in [72, Section 3.2]. In particular, if the errors in the measurements A and B are uncorrelated with zero mean and equal variance, then under mild conditions the classical TLS solution $\hat{X}$ of $AX \approx B$ is a strongly consistent estimate of the true solution X_0 of the corresponding unperturbed set $A_0X = B_0$ [26, 23; 72, Section 8.4].

Much of the literature concerns the *classical* TLS problem $AX \approx B$, in which all columns of A are subject to errors, but more general TLS problems, as well as other problems related to classical TLS, have been proposed and are being investigated (see [72] for a list of references).

First of all, in certain linear modeling problems *some* of the columns of A

may be *known exactly*. For instance, every intercept model

$$a + a_1 x_1 + \cdots + a_n x_n = b$$

gives rise to an overdetermined set of equations

$$[1_m; A]\begin{bmatrix}\alpha \\ x\end{bmatrix} = b$$

with $1_m = [1, \ldots, 1]^T$ in which the first column of the left-hand side matrix is known exactly [26, 28]. Other examples occur in system identification, for instance, when a system can be modeled as a transfer function model (see equation (43)). If the inputs to the system can be measured without error and enough input–output measurements are available, then estimating the parameters of these models gives rise to TLS problems with exactly known columns [70, 57].

In order to maximize the accuracy of the estimated parameters x, it is natural to require that the corresponding columns of A be unperturbed since they are known exactly. Therefore, the classical TLS problem formulation and the algorithms, as given in this paper, have been generalized. By varying the number of exactly known columns of $A_{m\times n}$ from 0 to n, this so-called *mixed LS–TLS* problem can handle the classical LS problem, any mixed TLS–LS problem and the classical TLS problem [72, Section 3.5; 28].

Moreover, the errors in the remaining data may be *correlated* and *not* equally sized. In order to maintain consistency of the result when solving these problems, the mixed LS–TLS problem formulation can be further *generalized* as follows (M^{-T} denotes the transposed inverse for matrix M).

DEFINITION 4 (*The generalized TLS (GTLS) problem*). Given a set of m linear equations in $n \times d$ unknowns X

$$AX \approx B\,, \quad A \in \mathbb{R}^{m\times n},\ B \in \mathbb{R}^{m\times d},\ \text{and } X \in \mathbb{R}^{n\times d}\,, \tag{44}$$

partition

$$A = [A_1; A_2]\,, \quad A_1 \in \mathbb{R}^{m\times n_1},\ A_2 \in \mathbb{R}^{m\times n_2},\ \text{and } n = n_1 + n_2\,, \tag{45}$$

$$X = [X_1^T; X_2^T]^T\,, \quad X_1 \in \mathbb{R}^{n_1\times d} \text{ and } X_2 \in \mathbb{R}^{n_2\times d} \tag{46}$$

and assume that the columns of A_1 are error-free and that nonsingular error equilibration matrices $D \in \mathbb{R}^{m\times m}$ and $C_2 \in R^{(n_2+d)\times(n_2+d)}$ are given such that the errors in $D^{-T}[A_2; B]C_2^{-1}$ are equilibrated, i.e., uncorrelated with zero mean and same variance. Then, the *generalized TLS (GTLS) problem* is the following:

$$\min_{[\hat{A}_2;\hat{B}]\in\mathbb{R}^{m\times(n_2+d)}} \|D^{-T}[A_2 - \hat{A}_2; B - \hat{B}]C_2^{-1}\|_F \tag{47}$$

$$\text{subject to} \quad R(\hat{B}) \subseteq R(\hat{A})\,. \tag{48}$$

Once a minimizing $[\hat{A}_2; \hat{B}]$ is found, then any $X = [X_1^T; X_2^T]^T$ satisfying

$$\hat{A}X = A_1X_1 + \hat{A}_2X_2 = \hat{B} \tag{49}$$

is called a *GTLS solution* and $[\Delta\hat{A}_2; \Delta\hat{B}] = [A_2 - \hat{A}_2; B - \hat{B}]$ the corresponding *generalized TLS correction*.

By varying n_1 from n to zero, this formulation can handle any LS ($n_1 = n$, $C_2 = I$, $D = I$) and generalized LS problem ($n_1 = n$, $C_2 = I$), as well as every TLS ($n_1 = 0$, $C_2 = I$, $D = I$), mixed LS–TLS ($C_2 = I$, $D = I$) and GTLS problem. If $D = I_m$ then C_2 is up to a factor of proportionality given by the square root of the error covariance matrix $\mathscr{C}_2 = \mathscr{E}([\Delta A_2; \Delta B]^T[\Delta A_2; \Delta B])$, which defines the correlations between the errors $[\Delta A_2; \Delta B]$ in $[A_2; B]$. Often, only $\mathscr{C}_2$ is known: in this case, the matrix C_2 is simply obtained from its Cholesky decomposition, i.e., $\mathscr{C}_2 = C_2^TC_2$ and C_2 upper triangular. Because of its close relation to the general EIV model, this special GTLS problem is of utmost importance in EIV regression. Indeed, under mild conditions the GTLS solution of this problem is shown to be a consistent estimate of the true parameters X_1^0, X_2^0 of this general EIV model. Consistency conditions for the one-dimensional GTLS solution ($d = 1$) are investigated by Gallo [25, 24] while Fuller [23, Section 4.1] proves consistency of the more general multidimensional GTLS solution. An algorithm which computes this GTLS solution by means of the GSVD, is outlined in [68]. Some further improvements in numerical performance are discussed in [81].

A further generalization of this GTLS problem, called the *restricted TLS* (*RTLS*) problem, is discussed in [73, 80, 82]. This formulation allows D and C to be rectangular, even rank-deficient any column of A and B can be declared error-fee and equality constraints can be imposed.

Other constrained TLS problems have been considered in literature. TLS problems subject to linear constraints are solved in [72, Section 10.2] while de Moor [19] investigated TLS problems $Ax \approx b$ with both nonnegativity constraints (i.e., $x \geqslant 0$) and inequality constraints $x \geqslant a, a \neq 0$ on the solution vector x.

Another constrained TLS problem has been formulated by Arun [10]. The problem addressed here and arising in signal processing applications, is the determination of the TLS solution $\hat{X}$ of $AX \approx B$, subject to the constraint that $\hat{X}$ be unitary. As proved by Arun, the solution to this *unitarily constrained TLS problem* is the same as the solution to the orthogonal Procrustes problem [32, p. 582].

Abatzoglou and Mendel [2] considered yet another constrained TLS problem, which extends the one-dimensional classical TLS problem $Ax \approx b$ to the case where the *errors* ΔA, Δb in the data A, b are *algebraically related*. In this case, the TLS solution may no longer yield optimal statistical estimators. This happens, for instance, in system identification when we try to estimate the impulse response of a system from its input and output by discrete deconvolu-

tion (see equation (42)). The errors in U are obviously Toeplitz and this information is not used in the classical TLS problem. To get more accurate estimates of $\hat{x}$, Abatzoglou and Mendel extended the classical TLS method to incorporate the algebraic dependence of the errors in $[A; b]$ and called their extension '*constrained TLS*'.

Another class of TLS related problems we consider here is obtained by formulating the classical TLS problem in some other norm. These problems, called *total approximation problems*, have been investigated by Späth, Watson and Osborne [75, 42, 53] and can be formulated as follows.

DEFINITION 5 (*Total approximation problem*). Find $\hat{x} \in \mathbb{R}^n$ to

$$\begin{aligned} &\text{minimize} && \|[\Delta A; \Delta b]\| \\ &\text{subject to} && (A + \Delta A)\hat{x} = b + \Delta b\,, \end{aligned} \tag{50}$$

where the norm $\|\cdot\|$ is an appropriate matrix norm.

For example, if the errors in A and b are independent and normally distributed then the most likely explanation of the data is achieved by minimizing the Frobenius norm of $[\Delta A; \Delta b]$, i.e., the classical TLS problem. However, if the data give rise to gross errors (wild points) then a more robust estimator may be the l_1 norm of the perturbation matrix regarded as an extended vector. For a situation between these two extremes, some other l_p norm, $1 < p < 2$, may be statistically more appropriate. (50) is a nonconvex problem, and so it may only be possible to find points satisfying first-order necessary conditions for local solutions (stationary points).

Finally, let us consider *nonlinear TLS* problems which arise from the fitting of observations (a_i, b_i), $i = 1, \ldots, m$ to a nonlinear model,

$$f(\alpha, x) = \beta\,. \tag{51}$$

In nonlinear regression the measurements a_i of the independent variable α are assumed to be exact and only the observations b_i of β are subject to random errors. In nonlinear TLS problems also the measurements of the independent variable α contain errors. Assume that a_i and b_i are subject to errors Δa_i and Δb_i respectively, so that

$$f(a_i - \Delta a_i, x) = b_i - \Delta b_i\,.$$

If the errors Δa_i and Δb_i are independent random variables with zero mean and equal variance, then it seems reasonable to choose the parameters x so that the sum of squares of the orthogonal distances $\sqrt{\Delta a_i^2 + \Delta b_i^2}$ from the observations (a_i, b_i) to the curve (51) is minimized. Hence the parameters x should be chosen as the solution to

$$\begin{aligned} &\min_{x, \Delta a, \Delta b} \sum_{i=1}^{m} (\Delta a_i^2 + \Delta b_i^2) \\ &\text{subject to} \quad f(a_i - \Delta a_i, x) = b_i - \Delta b_i\,, \quad i = 1, \ldots, m\,. \end{aligned}$$

Eliminating Δb_i using the constraints we arrive at the *orthogonal distance problem*

$$\min_{x,\Delta a} \sum_{i=1}^{m} \{(b_i - f(a_i - \Delta a_i, x))^2 + \Delta a_i^2\} .$$

If more generally $\alpha \in \mathbb{R}^n$ and $\beta \in \mathbb{R}^d$ in (51) are vectors, we have the problem

$$\min_{x,\Delta a} \sum_{i=1}^{m} \{\|b_i - f(a_i - \Delta a_i, x)\|_2^2 + \|\Delta a_i\|_2^2\} .$$

In particular when (51) reduces to $\alpha^T x = \beta$, $\beta \in \mathbb{R}$ and $x, \alpha \in \mathbb{R}^n$, the orthogonal distance problem is a classical TLS problem. Algorithms for the onlinear case, based on stabilized Gauss–Newton methods, have been given oy Schwetlick and Tiller [50, 51], Boggs, Byrd and Schnabel [13] and Golub and LeVeque [29] (see also [23, Section 3.2]).

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