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Overview of total least-squares methods

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Abstract

We review the development and extensions of the classical total least-squares method and describe algorithms for its generalization to weighted and structured approximation problems. In the generic case, the classical total least-squares problem has a unique solution, which is given in analytic form in terms of the singular value decomposition of the data matrix. The weighted and structured total least-squares problems have no such analytic solution and are currently solved numerically by local optimization methods. We explain how special structure of the weight matrix and the data matrix can be exploited for efficient cost function and first derivative computation. This allows to obtain computationally efficient solution methods. The total least-squares family of methods has a wide range of applications in system theory, signal processing, and computer algebra. We describe the applications for deconvolution, linear prediction, and errors-in-variables system identification.

Keywords: Total least squares; Orthogonal regression; Errors-in-variables model; Deconvolution; Linear prediction; System identification

1. Introduction

The total least-squares method was introduced by Golub and Van Loan [1,2] as a solution technique for an overdetermined system of equations $AX \approx B$, where $A \in \mathbb{R}^{m\times n}$ and $B \in \mathbb{R}^{m\times d}$ are the given data and $X \in \mathbb{R}^{n\times d}$ is unknown. With $m > n$, typically there is no exact solution for X, so that an approximate one is sought for. The total least-squares method is a natural generalization of the least-squares approximation method when the data in both A and B is perturbed.

The least-squares approximation $\widehat{X}_{\mathrm{ls}}$ is obtained as a solution of the optimization problem

$$\{\widehat{X}_{\mathrm{ls}}, \Delta B_{\mathrm{ls}}\} := \arg\min_{X,\Delta B} \|\Delta B\|_{\mathrm{F}} \quad \text{subject to } AX = B + \Delta B. \tag{LS}$$

The rationale behind this approximation method is to correct the right-hand side B as little as possible in the Frobenius norm sense, so that the corrected system of equations $AX = \widehat{B}$, $\widehat{B} := B + \Delta B$ has an exact solution. Under the condition that $\operatorname{vec} A$ is full column rank, the unique solution $\widehat{X}_{\mathrm{ls}} = (A^{\top}A)^{-1}A^{\top}B$ of the optimally corrected system of equations $AX = \widehat{B}_{\mathrm{ls}}$, $\widehat{B}_{\mathrm{ls}} := B + \Delta B_{\mathrm{ls}}$ is by definition the least-squares approximate solution of the original incompatible system of equations.

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Nomenclature

$\mathbb{R}$ and $\mathbb{R}_+$ the set of real numbers and non-negative real numbers
$:=$ and $:\Leftrightarrow$ left-hand side is defined by the right-hand side
$=:$ and $\Leftrightarrow:$ right-hand side is defined by the left-hand side
vec column-wise vectorization of a matrix
C, ΔC, $\widehat{C}$ data, correction, and approximation matrices
$C = [A \;\; B]$ input/output partitioning of the data
$c_1, \ldots, c_m$ observations, $[c_1 \;\; \cdots \;\; c_m] = C^\top$
$c = \mathrm{col}(a, b)$ the column vector $c = \left[\begin{smallmatrix} a \\ b \end{smallmatrix}\right]$
$\mathscr{B} \subseteq \mathbb{R}^{n+d}$ a static model in $\mathbb{R}^{n+d}$
$\mathscr{L}$ linear static model class
$\mathscr{B} \in \mathscr{L}_n$ linear static model of dimension at most n, i.e., a subspace (in $\mathbb{R}^{n+d}$) of dimension at most n
X, R, P parameters of input/output, kernel, and image representations
$\mathscr{B}_{\mathrm{i/o}}(X)$ input/output representation, see (I/O repr) in Section 3.1.3
$\mathrm{col\,span}(P)$ image representation, i.e., the space spanned by the columns of P
$\ker(R)$ kernel representation, i.e., the right null space of R

The definition of the total least-squares method is motivated by the asymmetry of the least-squares method: B is corrected while A is not. Provided that both A and B are given data, it is reasonable to treat them symmetrically. The classical total least-squares problem looks for the minimal (in the Frobenius norm sense) corrections ΔA and ΔB on the given data A and B that make the corrected system of equations $\widehat{A}X = \widehat{B}$, $\widehat{A} := A + \Delta A$, $\widehat{B} := B + \Delta B$ solvable, i.e.,

$$\{\widehat{X}_{\mathrm{tls}}, \Delta A_{\mathrm{tls}}, \Delta B_{\mathrm{tls}}\} := \arg \min_{X, \Delta A, \Delta B} \|[\Delta A \;\; \Delta B]\|_{\mathrm{F}} \quad \text{subject to } (A + \Delta A)X = B + \Delta B. \tag{TLS1}$$

The total least-squares approximate solution $\widehat{X}_{\mathrm{tls}}$ for X is a solution of the optimally corrected system of equations $\widehat{A}_{\mathrm{tls}}X = \widehat{B}_{\mathrm{tls}}$, $\widehat{A}_{\mathrm{tls}} := A + \Delta A_{\mathrm{tls}}$, $\widehat{B}_{\mathrm{tls}} := B + \Delta B_{\mathrm{tls}}$.

The least-squares approximation is statistically motivated as a maximum likelihood estimator in a linear regression model under standard assumptions (zero mean, normally distributed residual with a covariance matrix that is a multiple of the identity). Similarly, the total least-squares approximation is a maximum likelihood estimator in the errors-in-variables model

$$A = \bar{A} + \tilde{A}, \quad B = \bar{B} + \tilde{B} \text{ there exists an } \bar{X} \in \mathbb{R}^{n \times d} \text{ such that } \bar{A}\bar{X} = \bar{B} \tag{EIV}$$

under the assumption that vec $([\tilde{A} \;\; \tilde{B}])$ is a zero mean, normally distributed random vector with a covariance matrix that is a multiple of the identity. In the errors-in-variables (EIV) model, $\bar{A}$, $\bar{B}$ are the "true data", $\bar{X}$ is the "true" value of the parameter X, and $\tilde{A}$, $\tilde{B}$ consist of "measurement noise".

Our first aim is to review the development and generalizations of the total least-squares method. We start in Section 2 with an overview of the classical total least-squares method. Section 2.1 gives historical notes that relate the total least-squares method to work on consistent estimation in the EIV model. Section 2.2 presents the solution of the total least-squares problem and the resulting basic computational algorithm. Some properties, generalizations, and applications of the total least-squares method are stated in Sections 2.3–2.5.

Our second aim is to present an alternative formulation of the total least-squares problem as a matrix low rank approximation problem

$$\widehat{C}_{\mathrm{tls}} := \arg \min_{\widehat{C}} \|C - \widehat{C}\|_{\mathrm{F}} \quad \text{subject to } \mathrm{rank}(\widehat{C}) \leqslant n, \tag{TLS2}$$

which in some respects, described in detail later, has advantages over the classical one. With $C = [A \;\; B]$, the classical total least-squares problem (TLS1) is generically equivalent to the matrix low rank approximation problem (TLS2), however, in certain exceptional cases, known in the literature as non-generic total least-squares problems, (TLS1) fails to have a solution, while (TLS2) always has a solution.

The following example illustrates the geometry behind the least-squares and total least-squares approximations.

Example 1 (*Geometry of the least-squares and total least-squares methods*). Consider a data matrix $C = [a \;\; b]$ with $m = 20$ rows and $n + d = 2$ columns.

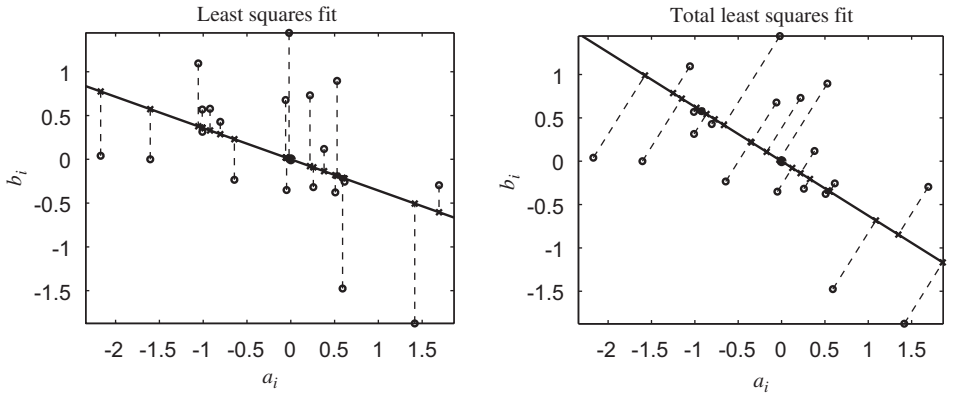

Fig. 1. Least-squares and total least-squares fits of a set of $m = 20$ data points in the plane. ○—data points $[a_i \;\; b_i]$, ×—approximations $[\widehat{a}_i \;\; \widehat{b}_i]$, solid line—fitting model $\widehat{a}\,\widehat{x} = \widehat{b}$, dashed lines—approximation errors.

The data are visualized in the plane: the rows $[a_i \;\; b_i]$ of C correspond to the circles in Fig. 1. Finding an approximate solution $\widehat{x}$ of the incompatible system of equations $ax \approx b$ amounts to fitting the data points by a *non-vertical* line passing through the origin. (The vertical line cannot be represented by an $x \in \mathbb{R}$.) The cases when the best fitting line happens to be vertical correspond to non-generic problems.

Alternatively, finding a rank-1 approximation $\widehat{C}$ of the given matrix C (refer to problem (TLS2)) amounts to fitting the data points $[a_i \;\; b_i]$ by points $[\widehat{a}_i \;\; \widehat{b}_i]$ (corresponding to the rows of $\widehat{C}$) that lie on a line passing through the origin. Note that now we do not exclude an approximation by the vertical line, because approximation points lying on a vertical line define a rank deficient matrix $\widehat{C}$ and problem (TLS2) does not impose further restrictions on the solution.

The least-squares and total least-squares methods assess the fitting accuracy in different ways: the least-squares method minimizes the sum of the squared vertical distances from the data points to the fitting line, while the total least-squares method minimizes the sum of the squared orthogonal distances from the data points to the fitting line. Fig. 1 shows the least-squares and total least-squares fitting lines as well as the data approximation (the crosses lying on the lines). In the least-squares case, the data approximation $\widehat{C}_{\mathrm{ls}} = [a \;\; b + \Delta b_{\mathrm{ls}}]$ is obtained by correcting the second coordinate only. In the total least-squares case, the data approximation $\widehat{C}_{\mathrm{tls}} = [a + \Delta a_{\mathrm{tls}} \;\; b + \Delta b_{\mathrm{tls}}]$ is obtained by correcting both coordinates.

In (TLS1) the constraint $\widehat{A}X = \widehat{B}$ *represents* the rank constraint $\mathrm{rank}(\widehat{C}) \leqslant n$, via the implication

$$\text{there exists an } X \in \mathbb{R}^{n\times d} \text{ such that } \widehat{A}X = \widehat{B} \quad \Rightarrow \quad \mathrm{rank}(\widehat{C}) \leqslant n, \quad \text{where} \quad \widehat{C} := [\widehat{A} \;\; \widehat{B}].$$

Note, however, that the reverse implication does not hold in general. This lack of equivalence is the reason for the existence of non-generic total least-squares problems. Problem (TLS1) is non-generic when the rank deficiency of $\widehat{C}_{\mathrm{tls}}$ (an optimal solution of (TLS2)) cannot be expressed as existence of linear relations $\widehat{A}X = \widehat{B}$ for some $X \in \mathbb{R}^{n\times d}$. In Section 3.1, we give an interpretation of the linear system of equations $\widehat{A}X = \widehat{B}$ as an input/output representation of a linear static model.

Apart from $\widehat{A}X = \widehat{B}$ with $\widehat{C} = [\widehat{A} \;\; \widehat{B}]$, there are numerous other ways to represent the rank constraint $\mathrm{rank}(\widehat{C}) \leqslant n$. For example, $\widehat{A}X = \widehat{B}$ with $\widehat{C}\Pi = [\widehat{A} \;\; \widehat{B}]$, where Π is an arbitrary permutation matrix, i.e., in (TLS2) we can choose to express any d columns of $\widehat{C}$ as a linear combination of the remaining columns in order to ensure rank deficiency of $\widehat{C}$. Any a priori fixed selection, however, leads to non-generic problems and therefore will be inadequate in certain cases. Of special importance are the kernel representation $R\widehat{C}^{\top} = 0$, where $RR^{\top} = I_d$, and the image representation $\widehat{C}^{\top} = PL$, where $P \in \mathbb{R}^{(n+d)\times n}$, $L \in \mathbb{R}^{n\times m}$. In contrast to the input/output representations, the kernel and image representations are equivalent to $\mathrm{rank}(\widehat{C}) \leqslant n$.

The representation-free total least-squares problem formulation (TLS2), described in Section 3, is inspired by the behavioral approach to system theory, put forward by Willems in the three part

remarkable paper [3]. We give an interpretation of the abstract rank condition as existence of a linear static model for the given data. Then:

> the total least squares method is viewed as a tool for deriving approximate linear static models.

This point of view is treated in more details for dynamic as well as static models in [4].

In Sections 3 and 5 we describe the extensions of the classical total least squares problem to weighted and structured total least-squares problems and classify the existing methods according to the representation of the rank constraint (input/output, kernel, or image) and the optimization method that is used for the solution of the resulting parameter optimization problem. We show that the block-Hankel structured total least-squares problem is a kernel problem for approximate modeling by a linear time-invariant dynamical model. Motivating examples are the deconvolution problem, the linear prediction problem, and the EIV system identification problem.

2. The classical total least-squares method

2.1. History

Although the name "total least squares" appeared only recently in the literature [1,2], this fitting method is not new and has a long history in the statistical literature where it is known as "orthogonal regression", "errors-in-variables", and "measurement errors". The univariate ($n = 1$, $d = 1$) problem is discussed already in 1877 by Adcock [5]. Latter on contributions are made by Adcock [6], Pearson [7], Koopmans [8], Madansky [9], and York [10]. The orthogonal regression method has been rediscovered many times, often independently. About 30 years ago, the technique was extended by Sprent [11] and Gleser [12] to multivariate ($n > 1$, $d > 1$) problems.

More recently, the total least-squares method also stimulated interest outside statistics. In the field of numerical analysis, this problem was first studied by Golub and Van Loan [1,2]. Their analysis, as well as their algorithm, is based on the singular value decomposition. Geometrical insight into the properties of the singular value decomposition brought Staar [13] independently to the same concept. Van Huffel and Vandewalle [14] 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 non-generic total least-squares problems and proved that the proposed generalization still satisfies the total least-squares criteria if additional constraints are imposed on the solution space. This seemingly different linear algebraic approach is actually equivalent to the method of multivariate EIV regression analysis, studied by Gleser [12]. Gleser's method is based on an eigenvalue–eigenvector analysis, while the total least-squares method uses the singular value decomposition which is numerically more robust in the sense of algorithmic implementation. Furthermore, the total least-squares algorithm computes the minimum norm solution whenever the total least-squares solution is not unique. These extensions are not considered by Gleser.

In engineering fields, e.g., experimental modal analysis, the total least-squares technique (more commonly known as the H_v technique), was also introduced about 20 years ago by Leuridan et al. [15]. In the field of system identification, Levin [16] first studied the problem. His method, called the eigenvector method or Koopmans–Levin method [17], computes the same estimate as the total least-squares algorithm whenever the total least-squares problem has a unique solution. Compensated least squares was yet another name arising in this area: this method compensates for the bias in the estimator, due to measurement error, and is shown by Stoica and Söderström [18] to be asymptotically equivalent to total least squares. Furthermore, in the area of signal processing, the minimum norm method Kumaresan and Tufts [19] was introduced and shown to be equivalent to minimum norm total least squares, see Dowling and Degroat [20]. Finally, the total least-squares approach is tightly related to the maximum likelihood principal component analysis method introduced in chemometrics by Wentzell et al. [21,22], see the discussion in Section 4.2.

The key role of least squares in regression analysis is the same as that of total least squares in EIV modeling. Nevertheless, a lot of confusion exists in the fields of numerical analysis and statistics about the principle of total least squares and its relation to EIV modeling. The computational advantages of total least squares are still largely unknown in the statistical community, while inversely the concept of EIV modeling did not penetrate sufficiently well in the field of computational mathematics and engineering.

A comprehensive description of the state of the art on total least squares from its conception up to the summer of 1990 and its use in parameter estimation has been presented in Van Huffel and Vandewalle [23]. While the latter book is entirely devoted to total least squares, a second [24] and third [25] edited books present the progress in total least squares and in the field of EIV modeling, respectively, from 1990 till 1996 and from 1996 till 2001.

2.2. Algorithm

The following theorem gives conditions for the existence and uniqueness of a total least-squares solution.

Theorem 2 (*Solution of the classical total least-squares problem*). *Let*

$$C := [A \;\; B] = U\Sigma V^\top \quad \text{where } \Sigma = \operatorname{diag}(\sigma_1, \ldots, \sigma_{n+d})$$

be a singular value decomposition of C, $\sigma_1 \geqslant \cdots \geqslant \sigma_{n+d}$ *be the singular values of* C, *and define the partitionings*

$$V := \begin{array}{c} \begin{matrix} n & d \end{matrix} \\ \begin{bmatrix} V_{11} & V_{12} \\ V_{21} & V_{22} \end{bmatrix} \end{array} \begin{array}{l} n \\ d \end{array} \quad \text{and} \quad \Sigma := \begin{array}{c} \begin{matrix} n & d \end{matrix} \\ \begin{bmatrix} \Sigma_1 & 0 \\ 0 & \Sigma_2 \end{bmatrix} \end{array} \begin{array}{l} n \\ d \end{array}.$$

A total least-squares solution exists if and only if V_{22} *is non-singular. In addition, it is unique if and only if* $\sigma_n \neq \sigma_{n+1}$. *In the case when the total least-squares solution exists and is unique, it is given by*

$$\widehat{X}_{\mathrm{tls}} = -V_{12}V_{22}^{-1}$$

and the corresponding total least-squares correction matrix is

$$\Delta C_{\mathrm{tls}} := [\Delta A_{\mathrm{tls}} \;\; \Delta B_{\mathrm{tls}}] = -U \operatorname{diag}(0, \Sigma_2) V^\top.$$

In the generic case when a unique total least-squares solution $\widehat{X}_{\mathrm{tls}}$ exists, it is computed from the d right singular vectors corresponding to the smallest singular values by normalization. This gives Algorithm 1 as a basic algorithm for solving the classical total least-squares problem (TLS1). Note that the total least-squares correction matrix ΔC_{tls} is such that the total least-squares data approximation

$$\widehat{C}_{\mathrm{tls}} := C + \Delta C_{\mathrm{tls}} = U \operatorname{diag}(\Sigma_1, 0) V^\top$$

is the best rank-n approximation of C.

Algorithm 1. Basic total least-squares algorithm.

Input: $A \in \mathbb{R}^{m\times n}$ and $B \in \mathbb{R}^{m\times d}$.
1: Compute the singular value decomposition $[A \;\; B] = U\Sigma V^\top$.
2: **if** V_{22} is non-singular **then**
3: Set $\widehat{X}_{\mathrm{tls}} = -V_{12}V_{22}^{-1}$.
4: **else**
5: Output a message that the problem (TLS1) has no solution and stop.
end if
Output: $\widehat{X}_{\mathrm{tls}}$—a total least-squares solution of $AX \approx B$.

Most total least-squares problems which arise in practice can be solved by Algorithm 1. Extensions of the basic total least-squares algorithm to problems in which the total least-squares solution does not exist or is not unique are considered in detail in [23]. In addition, it is shown how to speed up the total least-squares computations directly by computing the singular value decomposition only partially or iteratively if a good starting vector is available. More recent advances, e.g., recursive total least-squares algorithms, neural based total least-squares algorithms, rank-revealing total least-squares algorithms, total least-squares algorithms for large scale problems, etc., are reviewed in [24,25]. A novel theoretical and computational framework for treating non-generic and non-unique total least-squares problems is presented by Paige and Strakos [26].

2.3. Properties

Consider the EIV model and assume that $\operatorname{vec}([\tilde{A} \;\; \tilde{B}])$ is a zero mean random vector with a multiple of the identity covariance matrix. In addition, assume that $\lim_{m\to\infty} \tilde{A}^\top \tilde{A}/m$ exists and is a positive definite matrix. Under these assumptions it is proven [1,27] that the total least-squares solution $\widehat{X}_{\mathrm{tls}}$ is a weakly consistent estimator of the true parameter values $\bar{X}$, i.e.,

$$\widehat{X}_{\mathrm{tls}} \to \bar{X} \text{ in probability} \quad \text{as } m \to \infty.$$

This total least-squares property does not depend on the distribution of the errors. The total least-squares correction $[\Delta A_{\mathrm{tls}} \;\; \Delta B_{\mathrm{tls}}]$, however, being a rank d matrix is not an appropriate estimator for the measurement error matrix $[\tilde{A} \;\; \tilde{B}]$ (which is a full rank matrix with probability one). Note that the least-squares estimator $\widehat{X}_{\mathrm{ls}}$ is inconsistent in the EIV case.

In the special case of a single right-hand side ($d = 1$) and A full rank, the total least-squares problem has an analytic expression that is similar to the one of the least-squares solution

$$\text{least squares: } \widehat{x}_{\text{ls}} = (A^\top A)^{-1} A^\top b,$$
$$\text{total least squares: } \widehat{x}_{\text{tls}} = (A^\top A - \sigma_{n+1}^2 I)^{-1} A^\top b, \quad (*)$$

where σ_{n+1} is the smallest singular value of $[A\ b]$. From a numerical analyst's point of view, $(*)$ tells that the total least-squares solution is more ill-conditioned than the least-squares solution since it has a higher condition number. The implication is that errors in the data are more likely to affect the total least-squares solution than the least-squares solution. This is particularly true for the worst case perturbations. In fact, total least-squares is a *de*regularizing procedure. However, from a statistician's point of view, $(*)$ tells that the total least-squares method asymptotically removes the bias by subtracting the error covariance matrix (estimated by $\sigma_{n+1}^2 I$) from the data covariance matrix $A^\top A$.

While least-squares minimizes a sum of squared residuals, total least-squares minimizes a sum of *weighted* squared residuals:

$$\text{least squares: } \min_x \|Ax - b\|^2,$$
$$\text{total least squares: } \min_x \frac{\|Ax - b\|^2}{\|x\|^2 + 1}.$$

From a numerical analyst's point of view, total least-squares minimizes the Rayleigh quotient. From a statistician's point of view, total least-squares weights the residuals by multiplying them with the inverse of the corresponding error covariance matrix in order to derive a consistent estimate.

Other properties of total least squares, which were studied in the field of numerical analysis, are its sensitivity in the presence of errors on all data [23]. Differences between the least-squares and total least-squares solution are shown to increase when the ratio between the second smallest singular value of $[A\ b]$ and the smallest singular value of A is growing. In particular, this is the case when the set of equations $Ax \approx b$ becomes less compatible, the vector y is growing in length, or A tends to be rank-deficient. Assuming independent and identically distributed errors, the improved accuracy of the total least-squares solution compared to that of the least-squares solution is maximal when the orthogonal projection of b is parallel to the singular vector of A corresponding to the smallest singular value. Additional algebraic connections and sensitivity properties of the total least-squares and least-squares problems, as well as other statistical properties have been described in [23,24].

2.4. Extensions

The statistical model that corresponds to the basic total least-squares approach is the EIV model with the restrictive condition that the measurement errors are zero mean independent and identically distributed. In order to relax these restrictions, several extensions of the total least-squares problem have been investigated. The *mixed least-squares–total least-squares* problem formulation allows to extend consistency of the total least-squares estimator in EIV models, where some of the variables are measured without error. The *data least-squares* problem [28] refers to the special case in which the A matrix is noisy and the B matrix is exact. When the errors $[\tilde{A}\ \tilde{B}]$ are row-wise independent with equal row covariance matrix (which is known up to a scaling factor), the *generalized total least-squares* problem formulation [29] allows to extend consistency of the total least-squares estimator.

More general problem formulations, such as *restricted total least squares* [30], which also allow the incorporation of equality constraints, have been proposed, as well as total least-squares problem formulations using ℓ_p norms in the cost function. The latter problems, called *total ℓ_p approximations*, proved to be useful in the presence of outliers. Robustness of the total least-squares solution is also improved by adding regularization, resulting in *regularized total least-squares* methods [31–35]. In addition, various types of bounded uncertainties have been proposed in order to improve robustness of the estimators under various noise conditions [36,37].

Similarly to the classical total least-squares estimator, the generalized total least-squares estimator is computed reliably using the singular value decomposition. This is no longer the case for more general *weighted total least-squares* problems where the measurement errors are differently sized and/or correlated from row to row. Consistency of the weighted total least-squares estimator is proven and an iterative procedure for its computation is proposed in [38]. This problem is discussed in more detail in Section 3.

Furthermore, *constrained total least-squares* problems have been formulated. Arun [39] addressed

the unitarily constrained total least-squares problem, i.e., $AX \approx B$, subject to the constraint that the solution matrix X is unitary. He proved that this solution is the same as the solution to the orthogonal Procrustes problem [40, p. 582]. Abatzoglou et al. [41] considered yet another constrained total least-squares problem, which extends the classical total least-squares problem to the case where the errors $[\tilde{A}\ \tilde{B}]$ are algebraically related. In this case, the total least-squares solution is no longer statistically optimal (e.g., maximum likelihood in the case of normal distribution).

In the so-called *structured total least-squares* problems [42], the data matrix $[A\ B]$ is structured. In order to preserve the maximum likelihood properties of the solution, the total least-squares problem formulation is extended [43] with the additional constraint that the structure of the data matrix $[A\ B]$ is preserved in the correction matrix $[\Delta A\ \Delta B]$. Similarly to the weighted total least-squares problem, the structured total least-squares solution, in general, has no closed form expression in terms of the singular value decomposition. An important exception is the circulant structured total least squares, which can be solved using the fast Fourier transform, see [44]. In the general case, a structured total least-squares solution is searched via numerical optimization methods. However, efficient algorithms are proposed in the literature that exploit the matrix structure on the level of the computations. This research direction is further described in Section 5.

Regularized structured total least-squares solution methods are proposed in [45,46]. Regularization turns out to be important in the application of the structured total least-squares method for image deblurring [47–49]. In addition, solution methods for nonlinearly structured total least-squares methods are developed in [50,51].

2.5. Applications

Since the publication of the singular value decomposition based total least-squares algorithm [2], many new total least-squares algorithms have been developed and, as a result, the number of applications in total least squares and EIV modeling has increased in the last decade. Total least squares is applied in computer vision [52], image reconstruction [53–55], speech and audio processing [56,57], modal and spectral analysis [58,59], linear system theory [60,61], system identification [62–65], and astronomy [66]. An overview of EIV methods in system identification is given by Söderström in [67]. In [24,25], the use of total least squares and EIV models in the application fields are surveyed and new algorithms that apply the total least-squares concept are described.

A lot of common problems in system identification and signal processing can be reduced to special types of block-Hankel and block-Toeplitz structured total least-squares problems. In the field of signal processing, in particular in vivo magnetic resonance spectroscopy, and audio coding, new state-space based methods have been derived by making use of the total least-squares approach for spectral estimation with extensions to decimation and multichannel data quantification [68,69]. In addition, it has been shown how to extend the least mean squares algorithm to the EIV context for use in adaptive signal processing and various noise environments. Finally, total least-squares applications also emerge in other fields, including information retrieval [70], shape from moments [71], and computer algebra [72,73].

3. Representation-free total least-squares problem formulation

An insightful way of viewing the abstract rank constraint $\operatorname{rank}(C) \leqslant n$ is as the existence of a linear static model for C: $\operatorname{rank}(C) \leqslant n$ is equivalent to the existence of a subspace $\mathscr{B} \subset \mathbb{R}^{n+d}$ of dimension at most n that contains the rows of C.

> A subspace $\mathscr{B} \subseteq \mathbb{R}^{n+d}$ is referred to as a *linear static model*. Its dimension n is a measure of the model complexity: the higher the dimension the more complex and therefore less useful is the model $\mathscr{B}$.

The set of all linear static models of dimension at most n is denoted by $\mathscr{L}_n$. It is a non-convex set and has special properties that make it a Grassman manifold.

Let $[c_1\ \cdots\ c_m] := C^\top$, i.e., c_i is the transposed ith row of the matrix C and define the shorthand notation

$$C \in \mathscr{B} \subseteq \mathbb{R}^{n+d} \ :\Leftrightarrow\ c_i \in \mathscr{B} \quad \text{for } i = 1, \ldots, m.$$

We have the following equivalence

$$\operatorname{rank}(C) \leqslant n \ \Leftrightarrow\ C \in \mathscr{B} \in \mathscr{L}_n,$$

which relates the total least-squares problem (TLS2) to approximate linear static modeling. We restate

problem (TLS2) with this new interpretation and notation.

Problem 3 (*Total least squares*). Given a data matrix $C \in \mathbb{R}^{m\times(n+d)}$ and a complexity specification n, solve the optimization problem

$$\{\widehat{\mathscr{B}}_{\mathrm{tls}}, \widehat{C}_{\mathrm{tls}}\} := \arg \min_{\mathscr{B}\in\mathscr{L}_n} \min_{\widehat{C}\in\mathscr{B}} \|C - \widehat{C}\|_{\mathrm{F}}. \tag{TLS}$$

Note that (TLS) is a double minimization problem. On the inner level is the search for the best approximation of the given data C in a given model $\mathscr{B}$. The optimum value of this minimization

$$M_{\mathrm{tls}}(C, \mathscr{B}) := \min_{\widehat{C}\in\mathscr{B}} \|C - \widehat{C}\|_{\mathrm{F}} \tag{Mtls}$$

is a measure of the lack of fit between the data and the model and is called *misfit*. On the outer level is the search for the optimal model in the model class $\mathscr{L}_n$ of linear static models with bounded complexity. The optimality of the model is in terms of the total least-squares misfit function M_{tls}.

The double minimization structure, described above, is characteristic for all total least-squares problems. Since the model $\mathscr{B}$ is linear and the cost function is convex quadratic, the inner minimization can be solved analytically yielding a closed form expression for the misfit function. The resulting outer minimization, however, is a non-convex optimization problem and needs numerical solution methods. In the case of the basic total least-squares problem and the generalized total least-squares problem, presented in Section 3.3, the outer minimization can be brought back to a singular value decomposition computation. In more general cases, however, one has to rely on non-convex optimization methods and the guarantee to compute a global solution quickly and efficiently is lost.

In order to solve numerically the abstract total least-squares problem (TLS), we need to parameterize the fitting model. This important issue is discussed next.

3.1. Kernel, image, and input/output representations

As argued in the Introduction, the representation-free formulation is conceptually useful. For analysis, however, often it is more convenient to consider concrete representations of the model, which turn the abstract problem (TLS) into concrete parameter optimization problems, such as (TLS1). In this section, we present three representations of a linear static model: kernel, image, and input/output. They give different parameterizations of the model and are important in setting up algorithms for the solution of the problem.

3.1.1. Kernel representation

Let $\mathscr{B} \in \mathscr{L}_n$, i.e., $\mathscr{B}$ is an n-dimensional subspace of $\mathbb{R}^{n+d}$. A kernel representation of $\mathscr{B}$ is given by a system of equations $Rc = 0$, such that

$$\mathscr{B} = \{\, c \in \mathbb{R}^{n+d} \mid Rc = 0\} =: \ker(R).$$

The matrix $R \in \mathbb{R}^{g\times(n+d)}$ is a parameter of the model $\mathscr{B}$.

The parameter R is not unique. There are two sources for the non-uniqueness:

1. R might have redundant rows, and
2. for a full rank matrix U, $\ker(R) = \ker(UR)$.

The parameter R having redundant rows is related to the minimality of the representation. For a given linear static model $\mathscr{B}$, the representation $Rc = 0$ of $\mathscr{B}$ is minimal if R has the minimal number of rows among all parameters R that define a kernel representation of $\mathscr{B}$. The kernel representation, defined by R, is minimal if and only if R is full row rank.

Because of item 2, a minimal kernel representation is still not unique. All minimal representations, however, are related to a given one via a premultiplication of the parameter R with a non-singular matrix U. In a minimal kernel representation, the rows of R are a basis for $\mathscr{B}^{\perp}$, the orthogonal complement of $\mathscr{B}$, i.e.,

$$\mathscr{B}^{\perp} = \operatorname{row\,span}(R).$$

The choice of R is non-unique due to the non-uniqueness in the choice of basis of $\mathscr{B}^{\perp}$.

The minimal number of independent linear equations necessary to define a linear static model $\mathscr{B}$ is d, i.e., in a minimal representation $\mathscr{B} = \ker(R)$ with row $\dim(R) = d$.

3.1.2. Image representation

The dual of the kernel representation $\mathscr{B} = \ker(R)$ is the image representation

$$\mathscr{B} = \{c \in \mathbb{R}^{n+d} \mid c = Pl,\ l \in \mathbb{R}^n\} =: \operatorname{col\,span}(P).$$

Again for a given $\mathscr{B} \in \mathscr{L}_n$ an image representation $\mathscr{B} = \operatorname{col\,span}(P)$ is not unique because of possible non-minimality of P and the choice of basis. The representation is minimal if and only if P is

a full column rank matrix. In a minimal image representation, $\operatorname{col dim}(P) = \dim(\mathscr{B})$ and the columns of P form a basis for $\mathscr{B}$. Clearly $\operatorname{col span}(P) = \operatorname{col span}(PU)$, for any non-singular matrix $U \in \mathbb{R}^{n\times n}$. Note that

$$\ker(R) = \operatorname{col span}(P) = \mathscr{B} \in \mathscr{L}_n \;\Rightarrow\; RP = 0,$$

which gives a link between the parameters P and R.

3.1.3. Input/output representation

Both, the kernel and the image representations, treat all variables on an equal footing. In contrast, the more classical input/output representation

$$\mathscr{B}_{\mathrm{i/o}}(X) := \{c =: \operatorname{col}(a,b) \in \mathbb{R}^{n+d} \mid X^\top a = b\} \qquad \text{(I/O repr)}$$

distinguishes free variables $a \in \mathbb{R}^n$, called inputs, and dependent variables $b \in \mathbb{R}^d$, called outputs. In an input/output representation, a can be chosen freely, while b is fixed by a and the model. Note that for repeated observations $C^\top = [c_1 \;\cdots\; c_m]$ the statement $C \in \mathscr{B}_{\mathrm{i/o}}(X)$ is equivalent to the linear system of equations $AX = B$, where $[A\;\; B] := C$ with $A \in \mathbb{R}^{m\times n}$ and $B \in \mathbb{R}^{m\times d}$.

The partitioning $c = \operatorname{col}(a,b)$ gives an input/output partitioning of the variables: the first $n := \dim(a)$ variables are inputs and the remaining $d := \dim(b)$ variables are outputs. An input/output partitioning is not unique. Given a kernel or image representation, finding an input/output partitioning is equivalent to selecting a $d \times d$ full rank submatrix of R or an $n \times n$ full rank submatrix of P. In fact, generically, any splitting of the variables into a group of d variables (outputs) and a group of remaining variables (inputs), defines a valid input/output partitioning. In non-generic cases certain partitionings of the variables into inputs and outputs are not possible.

Note that in (I/O repr), the first n variables are fixed to be inputs, so that given X, the input/output represent $\mathscr{B}_{\mathrm{i/o}}(X)$ is fixed and vice versa, given $\mathscr{B} \in \mathscr{L}_n$, the parameter X (if it exists) is unique. Thus, as opposed to the parameters R and P in the kernel and the image representations, the parameter X in the input/output representation (I/O repr) is unique.

Consider the input/output $\mathscr{B}_{\mathrm{i/o}}(X)$, kernel $\ker(R)$, and image $\operatorname{col span}(P)$ representations of $\mathscr{B} \in \mathscr{L}_n$ and define the partitionings

$$R =: [R_{\mathrm{i}}\;\; R_{\mathrm{o}}], \quad R_{\mathrm{o}} \in \mathbb{R}^{d\times d} \quad \text{and}$$

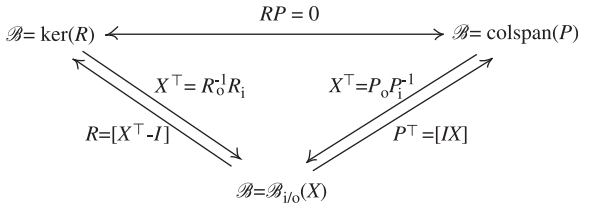

Fig. 2. Links among kernel, image, and input/output representations of $\mathscr{B} \in \mathscr{L}_n$.

$$P =: \begin{bmatrix} P_{\mathrm{i}} \\ P_{\mathrm{o}} \end{bmatrix}, \quad P_{\mathrm{i}} \in \mathbb{R}^{n\times n}.$$

The links among the parameters X, R, and P are summarized in Fig. 2.

3.2. Solution of the total least-squares problem

Approximation of the data matrix C with a model $\mathscr{B}$ in the model class $\mathscr{L}_n$ is equivalent to finding a matrix $\widehat{C} \in \mathbb{R}^{m\times(n+d)}$ with rank at most n. In the case when the approximation criterion is $\|C - \widehat{C}\|_{\mathrm{F}}$ (total least-squares problem) or $\|C - \widehat{C}\|_2$, the problem has a solution in terms of the singular value decomposition of C. The result is known as the Eckart–Young–Mirsky low-rank matrix approximation theorem [74]. We state it in the next lemma.

Lemma 4 (*Matrix approximation lemma*). *Let $C = U\Sigma V^\top$ be the singular value decomposition of $C \in \mathbb{R}^{m\times(n+d)}$ and partition the matrices U, $\Sigma =: \operatorname{diag}(\sigma_1, \ldots, \sigma_{n+d})$, and V as follows*:

$$U =: \begin{array}{c} \begin{matrix} n & d \end{matrix} \\ \begin{bmatrix} U_1 & U_2 \end{bmatrix} m \end{array}, \quad \Sigma =: \begin{array}{c} \begin{matrix} n & d \end{matrix} \\ \begin{bmatrix} \Sigma_1 & 0 \\ 0 & \Sigma_2 \end{bmatrix} \begin{matrix} n \\ d \end{matrix} \end{array} \quad \text{and}$$

$$V =: \begin{array}{c} \begin{matrix} n & d \end{matrix} \\ \begin{bmatrix} V_1 & V_2 \end{bmatrix} n + d. \end{array} \qquad \text{(SVD PRT)}$$

Then the rank-n matrix $\widehat{C}^* = U_1\Sigma_1 V_1^\top$ is such that

$$\|C - \widehat{C}^*\|_{\mathrm{F}} = \min_{\operatorname{rank}(\widehat{C}) \leqslant n} \|C - \widehat{C}\|_{\mathrm{F}} = \sqrt{\sigma_{n+1}^2 + \cdots + \sigma_{n+d}^2}.$$

The solution $\widehat{C}^*$ is unique if and only if $\sigma_{n+1} \neq \sigma_n$.

The solution of the total least-squares problem (TLS) trivially follows from Lemma 4.

Theorem 5 (*Solution of the total least-squares problem*). *Let $C = U\Sigma V^\top$ be the singular value*

decomposition of C and partition the matrices U, Σ, and V as in (SVD PRT). *Then a total least-squares approximation of C in $\mathscr{L}_n$ is*

$$\widehat{C}_{\mathrm{tls}} = U_1\Sigma_1 V_1^\top, \quad \widehat{\mathscr{B}}_{\mathrm{tls}} = \ker(V_2^\top) = \operatorname{col\,span}(V_1),$$

and the total least-squares misfit is

$$M_{\mathrm{tls}}(C,\mathscr{B}) = \|\Sigma_2\|_{\mathrm{F}} = \sqrt{\sigma_{n+1}^2 + \cdots + \sigma_{n+d}^2} \quad \text{where}$$
$$\Sigma_2 =: \operatorname{diag}(\sigma_{n+1},\ldots,\sigma_{n+d}).$$

A total least-squares approximation always exists. It is unique if and only if $\sigma_n \neq \sigma_{n+1}$.

Note 6 (*Non-generic total least-squares problems*). The optimal approximating model $\widehat{\mathscr{B}}_{\mathrm{tls}}$ might have no input/output representation (I/O repr). In this case, the optimization problem (TLS1) has no solution. By suitable permutation of the variables, however, (TLS1) can be made solvable, so that $\widehat{X}_{\mathrm{tls}}$ exists and $\widehat{\mathscr{B}}_{\mathrm{tls}} = \mathscr{B}_{\mathrm{i/o}}(\widehat{X}_{\mathrm{tls}})$.

The issue of whether the total least-squares problem is generic or not is not related to the approximation of the data per se but to the possibility of representing the optimal model $\widehat{\mathscr{B}}_{\mathrm{tls}}$ in the form (I/O repr), i.e., to the possibility of imposing a *given* input/output partition on $\widehat{\mathscr{B}}_{\mathrm{tls}}$.

3.3. Generalized total least-squares problem

Let $W_\ell \in \mathbb{R}^{m\times m}$ and $W_{\mathrm{r}} \in \mathbb{R}^{(n+d)\times(n+d)}$ be given positive definite matrices and define the following generalized total least-squares misfit function

$$M_{\mathrm{gtls}}(C,\mathscr{B}) = \min_{\widehat{C}\in\mathscr{B}} \|\sqrt{W_\ell}(C-\widehat{C})\sqrt{W_{\mathrm{r}}}\|_{\mathrm{F}}. \tag{Mgtls}$$

(W_ℓ allows for a row weighting and W_{r} for a column weighting in the cost function.) The resulting approximation problem is called generalized total least-squares problem.

Problem 7 (*Generalized total least squares*). Given a data matrix $C \in \mathbb{R}^{m\times(n+d)}$, positive definite weight matrices W_ℓ and W_{r}, and a complexity specification n, solve the optimization problem

$$\{\widehat{\mathscr{B}}_{\mathrm{gtls}}, \widehat{C}_{\mathrm{gtls}}\} = \arg\min_{\widehat{\mathscr{B}}\in\mathscr{L}_n} M_{\mathrm{gtls}}(C,\mathscr{B}). \tag{GTLS}$$

The solution of the generalized total least-squares problem can be obtained from the solution of a total least-squares problem for a modified data matrix.

Theorem 8 (*Solution of the generalized total least-squares problem*). *Define the modified data matrix*

$$C_{\mathrm{m}} := \sqrt{W_\ell}\,C\,\sqrt{W_{\mathrm{r}}},$$

and let $\widehat{C}_{\mathrm{m,tls}}$, $\widehat{\mathscr{B}}_{\mathrm{m,tls}} = \ker(R_{\mathrm{m,tls}}) = \operatorname{col\,span}(P_{\mathrm{m,tls}})$ be a total least-squares approximation of C_{m} in $\mathscr{L}_n$. Then a solution of the generalized total least-squares problem (GTLS) *is*

$$\widehat{C}_{\mathrm{gtls}} = (\sqrt{W_\ell})^{-1}\widehat{C}_{\mathrm{m,tls}}(\sqrt{W_{\mathrm{r}}})^{-1},$$

$$\widehat{\mathscr{B}}_{\mathrm{gtls}} = \ker(R_{\mathrm{m,tls}}\sqrt{W_{\mathrm{r}}}) = \operatorname{col\,span}((\sqrt{W_{\mathrm{r}}})^{-1}P_{\mathrm{m,tls}})$$

and the corresponding generalized total least-squares misfit is $M_{\mathrm{gtls}}(C,\mathscr{B}_{\mathrm{gtls}}) = M_{\mathrm{tls}}(C_{\mathrm{m}},\mathscr{B}_{\mathrm{m,tls}})$. A generalized total least-squares solution always exists. It is unique if and only if $\widehat{\mathscr{B}}_{\mathrm{m,tls}}$ is unique.

Robust algorithms for solving the generalized total least-squares problem without explicitly computing the inverses $(\sqrt{W_\ell})^{-1}$ and $(\sqrt{W_{\mathrm{r}}})^{-1}$ are proposed in [29,30,75]. These algorithms give better accuracy when the weight matrices are nearly rank deficient. In addition, they can treat the singular case, which implies that some rows and/or columns of C are considered exact and are not modified in the solution $\widehat{C}$.

If the matrices W_ℓ and W_{r} are diagonal, i.e., $W_\ell = \operatorname{diag}(w_{\ell,1},\ldots,w_{\ell,m})$, where $w_\ell \in \mathbb{R}_+^m$ and $W_{\mathrm{r}} = \operatorname{diag}(w_{\mathrm{r},1},\ldots,w_{\mathrm{r},n+d})$, where $w_{\mathrm{l}} \in \mathbb{R}_+^{n+d}$ the generalized total least-squares problem is called *scaled total least-squares*.

4. Weighted total least squares

For a given positive definite weight matrix $W \in \mathbb{R}^{m(n+d)\times m(n+d)}$ define the weighted matrix norm

$$\|C\|_W := \sqrt{\operatorname{vec}^\top(C^\top)W\operatorname{vec}(C^\top)}$$

and the weighted total least-squares misfit function

$$M_{\mathrm{wtls}}(C,\mathscr{B}) := \min_{\widehat{C}\in\mathscr{B}} \|C-\widehat{C}\|_W. \tag{Mwtls}$$

The approximation problem with weighted total least-squares misfit function is called the weighted total least-squares problem.

Problem 9 (*Weighted total least squares*). Given a data matrix $C \in \mathbb{R}^{m\times(n+d)}$, a positive definite weight matrix W, and a complexity specification n, solve the optimization problem

$$\{\widehat{\mathscr{B}}_{\mathrm{wtls}}, \widehat{C}_{\mathrm{wtls}}\} := \arg\min_{\widehat{\mathscr{B}}\in\mathscr{L}_n} M_{\mathrm{wtls}}(C,\mathscr{B}). \tag{WTLS}$$

The motivation for considering the weighted total least-squares problem is that it defines the maximum likelihood estimator for the EIV model when the measurement noise $\tilde{C} = [\tilde{A}\ \tilde{B}]$ is zero mean, normally distributed, with a covariance matrix

$$\operatorname{cov}(\operatorname{vec}(\tilde{C}^\top)) = \sigma^2 W^{-1}, \qquad (**)$$

i.e., the weight matrix W is up to a scaling factor σ^2 the inverse of the measurement noise covariance matrix.

Note 10 (*Element-wise weighted total least-squares*). The special case when the weight matrix W is diagonal is called element-wise weighted total least squares. It corresponds to an EIV problem with uncorrelated measurement errors. Let $W = \operatorname{diag}(w_1, \ldots, w_{m(n+d)})$ and define the $m \times (n+d)$ weight matrix Σ by $\Sigma_{ij} := w_{(i-1)(n+d)+j}$. Denote by $\odot$ the element-wise product $A \odot B = [a_{ij} b_{ij}]$. Then

$$\|\Delta C\|_W = \|\Sigma \odot \Delta C\|_{\mathrm{F}}.$$

Note 11 (*Total least squares as an unweighted weighted total least squares*). The extreme special case when $W = I$ is called unweighted. Then the weighted total least-squares problem reduces to the total least-squares problem. The total least-squares misfit M_{tls} weights equally all elements of the correction matrix ΔC. It is a natural choice when there is no prior knowledge about the data. In addition, the unweighted case is computationally easier to solve than the general weighted case.

Special structure of the weight matrix W results in special weighted total least-squares problems. Fig. 3 shows a hierarchical classification of various problems considered in the literature. From top to bottom the generality of the problems decreases: on the top is a weighted total least-squares problem for a general positive semi-definite weight matrix and on the bottom is the classical total least-squares problem. In between are weighted total least-squares problems with (using the stochastic terminology) uncorrelated errors among the rows, among the columns, and among all elements (element-wise weighted total least-squares case). Row-wise and column-wise uncorrelated weighted total least-squares problems, in which the row or column weight matrices are equal are generalized total least-squares problems with, respectively, $W_\ell = I$ and $W_{\mathrm{r}} = I$. In order to express easily the structure of the weight matrix in the case of column-wise uncorrelated errors, we introduce the weight matrix $\bar{W}$ as follows: $\operatorname{cov}(\operatorname{vec}(\tilde{C})) = \sigma^2 \bar{W}^{-1}$, compare with (**), where $\tilde{C}$ is transposed.

With $W = I$, (WTLS) coincides with the total least-squares problem (TLS). Except for the special case of generalized total least squares, however, the weighted total least-squares problem has no closed form solution in terms of the singular value decomposition. As an optimization problem it is non-convex, so that the currently available solution methods do not guarantee convergence to a global optimum solution. In the rest of this section, we give an overview of solution methods for the weighted total least-squares problem, with emphasis on the row-wise weighted total least-squares case, i.e., when the weight matrix W is block diagonal $W = \operatorname{diag}(W_1, \ldots, W_m)$, $W_i \in \mathbb{R}^{(n+d)\times(n+d)}$, $W_i > 0$. In the EIV setting, this assumption implies that the measurement errors $\tilde{c}_i$ and $\tilde{c}_j$ are uncorrelated for all $i, j = 1, \ldots, m$, $i \neq j$, which is a reasonable assumption for most applications.

Similarly to the total least-squares and generalized total least-squares problems, the weighted total least-squares problem is a double minimization problem. The inner minimization is the search for the best approximation of the data in a given model and an outer minimization is the search for the model. First, we solve the inner minimization problem—the misfit computation.

4.1. Best approximation of the data by a given model

Since the model is linear, (Mwtls) is a convex optimization problem with an analytic solution. In order to give explicit formulas for the optimal approximation $\widehat{C}_{\mathrm{wtls}}$ and misfit $M_{\mathrm{wtls}}(C, \mathscr{B})$, however, we need to choose a particular parameterization of the given model $\mathscr{B}$. We state the results for the kernel and the image representations. The results for the input/output representation follow from the given ones by the substitutions $R \mapsto [X^\top\ -I]$ and $P \mapsto \left[\begin{smallmatrix} I \\ X^\top \end{smallmatrix}\right]$.

Theorem 12 (*Weighted total least-squares misfit computation, kernel representation version*). *Let* $\ker(R)$ *be a minimal kernel representation of* $\mathscr{B} \in \mathscr{L}_n$. *The best weighted total least-squares approximation of* C *in* $\mathscr{B}$, *i.e., the solution of* (Mwtls), *is*

$$\widehat{c}_{\mathrm{wtls},i} = (I - W_i^{-1} R^\top (R W_i^{-1} R^\top)^{-1} R) c_i \quad \text{for } i = 1, \ldots, m$$

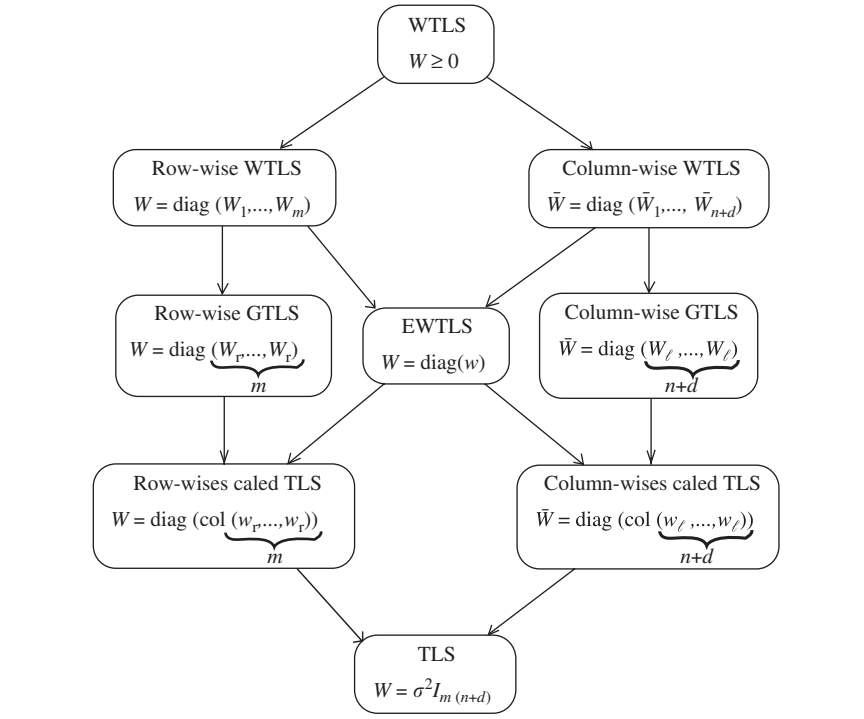

Fig. 3. Hierarchy of weighted total least-squares problems according to the structure of the weight matrix W. On the left side are weighted total least-squares problems with row-wise uncorrelated measurement errors and on the right side are weighted total least-squares problems with column-wise uncorrelated measurement errors.

with the corresponding misfit

$$M_{\text{wtls}}(C, \ker(R)) = \sqrt{\sum_{i=1}^{m} c_i^\top R^\top (R W_i^{-1} R^\top)^{-1} R c_i}. \qquad (\text{Mwtls}_R)$$

The image representation is dual to the kernel representation. Correspondingly, the misfit computation with kernel and with image representations of the model are dual problems. The kernel representation leads to a least norm problem and the image representation leads to a least-squares problem.

Theorem 13 (*Weighted total least-squares misfit computation, image representation version*). *Let* $\text{col span}(P)$ *be a minimal image representation of* $\mathscr{B} \in \mathscr{L}_n$. *The best weighted total least-squares approximation of* C *in* $\mathscr{B}$ *is*

$$\widehat{c}_{\text{wtls},i} = P(P^\top W_i P)^{-1} P^\top W_i c_i \quad \text{for } i = 1,\ldots,m$$

with the corresponding misfit

$$M_{\text{wtls}}(C, \text{col span}(P)) = \sqrt{\sum_{i=1}^{m} c_i^\top W_i (I - P(P^\top W_i P)^{-1} P^\top W_i) c_i}. \qquad (\text{Mwtls}_P)$$

4.2. Optimization over the model parameters

The remaining problem—the minimization with respect to the model parameters is a non-convex optimization problem that in general has no closed form solution. For this reason numerical optimization methods are employed for its solution.

Special optimization methods for the weighted total least-squares problem are proposed in [21,42,76–78]. The Riemannian singular value decomposition framework of De Moor [42] is derived for the structured total least-squares problem but

includes the weighted total least-squares problem with diagonal weight matrix and $d = 1$ as a special case. The restriction to more general weighted total least-squares problems comes from the fact that the Riemannian singular value decomposition framework is derived for matrix approximation problems with rank reduction by one. De Moor proposed an algorithm resembling the inverse power iteration algorithm for computing the solution. The method, however, has no proven convergence properties.

The maximum likelihood principle component analysis method of Wentzell et al. [21] is an alternating least-squares algorithm. It applies to the general weighted total least-squares problems and is globally convergent, with linear convergence rate. The method of Premoli and Rastello [76] is a heuristic for solving the first order optimality condition of (WTLS). A solution of a nonlinear equation is sought instead of a minimum point of the original optimization problem. The method is locally convergent with superlinear convergence rate. The region of convergence around a minimum point could be rather small in practice. The weighted low rank approximation framework of Manton et al. [78] proposes specialized optimization methods on a Grassman manifold. The least-squares nature of the problem is not exploited by the algorithms proposed in [78].

The Riemannian singular value decomposition, maximum likelihood principle component analysis, Premoli–Rastello, and weighted low rank approximation methods differ in the parameterization of the model and the optimization algorithm used, see Table 1.

Table 1
Model representations and optimization algorithms used in the methods of [21,22,42,76,78]

Method	Representation	Algorithm
Riemannian singular value decomposition	Kernel	Inverse power iteration
Maximum likelihood principle component analysis	Image	Alternating projections
Premoli–Rastello	Input/output	Iteration based on heuristic linearization
Weighted low rank approximation	Kernel	Newton method

5. Structured total least squares

The total least-squares problem is a tool for approximate modeling by a static linear model. Similarly, the structured total least-squares problem with block-Hankel structured data matrix is a tool for approximate modeling by a linear time-invariant dynamic model. In order to show how the block-Hankel structure occurs, consider a difference equation represented by an linear time-invariant model

$$R_0 w_t + R_1 w_{t+1} + \cdots + R_l w_{t+l} = 0. \qquad \text{(KER)}$$

Here $R_0, \ldots, R_l$ are the model parameters and the integer l is the *lag* of the equation. For $t = 1, \ldots, T - l$, the difference equation (KER) is equivalent to the block-Hankel structured system of equations

$$[\, R_0 \quad R_1 \quad \cdots \quad R_l \,] \underbrace{\begin{bmatrix} w_1 & w_2 & \cdots & w_{T-l} \\ w_2 & w_3 & \cdots & w_{T-l+1} \\ \vdots & \vdots & & \vdots \\ w_{l+1} & w_{l+2} & \cdots & w_T \end{bmatrix}}_{\mathscr{H}_l(w)} = 0. \qquad \text{(Hank eqn)}$$

Thus the constraint that a time series $w = (w(1), \ldots, w(T))$ is a trajectory of the linear time-invariant model implies rank deficiency of the block-Hankel matrix $\mathscr{H}_l(w)$.

Next we show three typical examples that illustrate the occurrence of structured system of equations in approximate modeling problems.

5.1. Examples

5.1.1. Deconvolution

The convolution of the (scalar) sequences

$$(\ldots, a_{-1}, a_0, a_1, \ldots) \quad \text{and} \quad (\ldots, x_{-1}, x_0, x_1, \ldots)$$

is the sequence $(\ldots, b_{-1}, b_0, b_1, \ldots)$ defined as follows:

$$b_i = \sum_{j=-\infty}^{\infty} x_j a_{i-j}. \qquad \text{(CONV)}$$

Assume that $x_j = 0$ for all $j < 1$ and for all $j > n$. Then (CONV) for $i = 1, \ldots, m$ can be written as the

following structured system of equations:

$$\underbrace{\begin{bmatrix} a_0 & a_{-1} & \cdots & a_{1-n} \\ a_1 & a_0 & \cdots & a_{2-n} \\ \vdots & \vdots & & \vdots \\ a_{m-1} & a_{m+n-2} & \cdots & a_{m-n} \end{bmatrix}}_{A} \underbrace{\begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}}_{x} = \underbrace{\begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_m \end{bmatrix}}_{b}. \tag{CONV′}$$

Note that the matrix A is Toeplitz structured and is parameterized by the vector $a = \mathrm{col}(a_{1-n}, \ldots, a_{m-1}) \in \mathbb{R}^{m+n-1}$.

The aim of the deconvolution problem is to find x, given a and b. With exact data the problem boils down to solving the system of equations (CONV′). By construction it has an exact solution. Moreover the solution is unique whenever A is of full column rank, which can be translated to a persistency of excitation condition on a, see [79].

The deconvolution problem is more realistic and more challenging when the data a, b are perturbed. We assume that $m > n$, so that the system of equations (CONV′) is overdetermined. Because both a and b are perturbed and the A matrix is structured, the deconvolution problem is a total least-squares problem with structured data matrix $C = [A\ b]$, A Toeplitz and b unstructured.

5.1.2. Linear prediction

In many signal processing applications the sum of damped exponentials model

$$\widehat{y}_t = \sum_{i=1}^{l} c_i \mathrm{e}^{d_i t} \mathrm{e}^{\mathbf{i}(\omega_i t + \phi_i)} \quad \text{where } \mathbf{i} := \sqrt{-1} \tag{SDE}$$

is considered. Given an observed sequence $(y_{\mathrm{d},1}, \ldots, y_{\mathrm{d},T})$ ("d" stands for data), the aim is to find parameters $\{c_i, d_i, \omega_i, \phi_i\}_{i=1}^{l}$ of a sum of damped exponentials model, such that the signal $\widehat{y}$ given by (SDE) is close to the observed one, e.g.,

$$\min \left\| \begin{bmatrix} y_{\mathrm{d},1} \\ \vdots \\ y_{\mathrm{d},T} \end{bmatrix} - \begin{bmatrix} \widehat{y}_1 \\ \vdots \\ \widehat{y}_T \end{bmatrix} \right\|.$$

Note that the sum of damped exponentials model is just an autonomous linear time-invariant model, i.e., $\widehat{y}$ is a free response of an linear time-invariant system. Therefore $\widehat{y}$ satisfies a homogeneous linear difference equation

$$\widehat{y}_t + \sum_{\tau=1}^{l} a_\tau \widehat{y}_{t+\tau} = 0. \tag{LP}$$

Approximating y_{d} by a signal $\widehat{y}$ that satisfies (LP) is a linear prediction problem, so modeling y_{d} as a sum of damped exponentials is equivalent to the linear prediction problem. Of course, there is a one-to-one relation between the initial conditions $\widehat{y}_0, \ldots, \widehat{y}_{-l+1}$ and parameters $\{a_i\}_{i=1}^{l}$ of (LP) and the parameters $\{c_i, d_i, \omega_i, \phi_i\}_{i=1}^{l}$ of (SDE).

For a time horizon $t = 1, \ldots, T$, with $T > l + 1$, (LP) can be written as the structured system of equations

$$\begin{bmatrix} \widehat{y}_1 & \widehat{y}_2 & \cdots & \widehat{y}_l \\ \widehat{y}_2 & \widehat{y}_3 & \cdots & \widehat{y}_{l+1} \\ \vdots & \vdots & & \vdots \\ \widehat{y}_m & \widehat{y}_{m+1} & \cdots & \widehat{y}_{T-1} \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \\ \vdots \\ a_l \end{bmatrix} = - \begin{bmatrix} \widehat{y}_{l+1} \\ \widehat{y}_{l+2} \\ \vdots \\ \widehat{y}_T \end{bmatrix},$$

where $m := T - l$. Therefore, the Hankel matrix $\mathscr{H}_{l+1}(\widehat{y})$ with $l + 1$ columns, constructed from $\widehat{y}$ is rank deficient. Conversely, if $\mathscr{H}_{l+1}(\widehat{y})$ has a one-dimensional left kernel, then $\widehat{y}$ satisfies the linear recursion (LP). Therefore, the linear prediction problem is the problem of finding the smallest in some sense (e.g., 2-norm) correction Δy on the given sequence y_{d} that makes a block-Hankel matrix $\mathscr{H}_{l+1}(\widehat{y})$ constructed from the corrected sequence $\widehat{y} := y_{\mathrm{d}} - \Delta y$ rank deficient. This is an structured total least-squares problem $Ax \approx b$ with Hankel structured data matrix $C = [A\ b]$.

5.1.3. EIV identification

Consider the linear time-invariant system described by the difference equation

$$\widehat{y}_t + \sum_{\tau=1}^{l} a_\tau \widehat{y}_{t+\tau} = \sum_{\tau=0}^{l} b_\tau \widehat{u}_{t+\tau} \tag{DE}$$

and define the parameter vector

$$x := \mathrm{col}(b_0, \ldots, b_l, -a_0, \ldots, -a_{l-1}) \in \mathbb{R}^{2l+1}.$$

Given a set of input/output data $(u_{\mathrm{d},1}, y_{\mathrm{d},1}), \ldots, (u_{\mathrm{d},T}, y_{\mathrm{d},T})$ and an order specification l, we want to find the parameter x of a system that fits the data.

For a time horizon $t = 1, \ldots, T$, (DE) can be written as the structured system of equations

$$\left[\begin{array}{cccc|ccc} \widehat{u}_1 & \widehat{u}_2 & \cdots & \widehat{u}_{l-1} & \widehat{y}_1 & \widehat{y}_2 & \cdots & \widehat{y}_l \\ \widehat{u}_2 & \widehat{u}_3 & \cdots & \widehat{u}_{l+2} & \widehat{y}_2 & \widehat{y}_3 & \cdots & \widehat{y}_{l+1} \\ \vdots & \vdots & & \vdots & \vdots & \vdots & & \vdots \\ \widehat{u}_m & \widehat{u}_{m+1} & \cdots & \widehat{u}_T & \widehat{y}_m & \widehat{y}_{m+1} & \cdots & \widehat{y}_{T-1} \end{array}\right] x = \left[\begin{array}{c} \widehat{y}_{l+1} \\ \widehat{y}_{l+2} \\ \vdots \\ \widehat{y}_T \end{array}\right], \tag{DE$'$}$$

where $m := T - l$. We assume that the time horizon is large enough to ensure $m > 2l + 1$. The system (DE$'$) is satisfied for exact data and a solution is the true value of the parameter x. Moreover, under additional assumption on the input (persistency of excitation) the solution is unique.

For perturbed data an approximate solution is sought and the fact that the system of equation (DE$'$) is structured suggests the use of the structured total least-squares method. Under appropriate conditions for the data generating mechanism an structured total least-squares solution provides a maximum likelihood estimator. The structure arising in the EIV identification problem is $C = [\mathscr{H}_l^\top(u_\mathrm{d}) \;\; \mathscr{H}_l^\top(y_\mathrm{d})]$.

5.2. History of the structured total least-squares problem

The origin of the structured total least-squares problem dates back to the work of Aoki and Yue [80], although the name "structured total least-squares" appeared only 23 years later in the literature [42]. Aoki and Yue consider a single input single output system identification problem, where both the input and the output are noisy (EIV setting) and derive a maximum likelihood solution. Under the normality assumption for the measurement errors, a maximum likelihood estimate turns out to be a solution of the structured total least-squares problem. Aoki and Yue approach the optimization problem in a similar way to the one presented in Section 5.3: they use classical nonlinear least-squares minimization methods for solving an equivalent unconstrained problem.

The structured total least-squares problem occurs frequently in signal processing applications. Cadzow [81], Bresler and Macovski [82] propose heuristic solution methods that turn out to be *suboptimal* with respect to the ℓ_2-optimality criterion, see Tufts and Shah [83] and De Moor [61, Section V]. These methods, however, became popular because of their simplicity. For example, the method of Cadzow is an iterative method that alternates between unstructured low rank approximation and structure enforcement, thereby only requiring singular value decomposition computations and manipulation of the matrix entries.

Tufts and Shah propose in [83], a *non-iterative* method for Hankel structured total least-squares approximation that is based on perturbation analysis and provides nearly optimal solution for high signal-to-noise ratio (SNR). In a statistical setting, this method achieves the Cramer–Rao lower bound asymptotically as the SNR tends to infinity. Non-iterative methods for solving the linear prediction problem (which, as shown in Section 5.1, is equivalent to Hankel structured total least-squares problem) are proposed by Tufts and Kumaresan in their seminal work [84,85].

Abatzoglou et al. [41] are considered to be the first who formulated a structured total least-squares problem. They called their approach constrained total least squares and motivate the problem as an extension of the total least-squares method to matrices with structure. The solution approach adopted by Abatzoglou et al. is closely related to the one of Aoki and Yue. Again an equivalent optimization problem is derived, but it is solved numerically using a Newton-type optimization method.

Shortly after the publication of the work on the constrained total least-squares problem, De Moor [42] lists many applications of the structured total least-squares problem and outlines a new framework for deriving analytical properties and numerical methods. His approach is based on the Lagrange multipliers and the basic result is an equivalent problem, called Riemannian singular value decomposition, which can be considered as a "nonlinear" extension of the classical singular value decomposition. As an outcome of the new problem formulation, an iterative solution method based on the inverse power iteration is proposed.

Another algorithm for solving the structured total least-squares problem (even with ℓ_1 and ℓ_∞ norm in the cost function), called structured total least norm, is proposed by Rosen et al. [86]. In contrast to the approaches of Aoki, Yue and Abatzoglou et al., Rosen et al. solve the problem in its original formulation. The constraint is linearized around the current iteration point, which results in a linearly constrained least-squares problem. In the algorithm of Rosen et al., the constraint is incorporated in the

cost function by adding a multiple of its residual norm.

The weighted low rank approximation framework of Manton et al. [78] has been extended in [87,88] to structured low rank approximation problems. All problem formulations and solution methods cited above, except for the ones in the structured low rank approximation framework, aim at rank reduction of the data matrix C by one. A generalization of the algorithm of Rosen et al. to problems with rank reduction by more than one is proposed by Van Huffel et al. [89]. It involves, however, Kronecker products that unnecessary inflate the dimension of the involved matrices.

When dealing with a general affine structure the constrained total least squares, Riemannian singular value decomposition, and structured total least norm methods have cubic computational complexity per iteration in the number of measurements. Fast algorithms with linear computational complexity are proposed by Mastronardi et al. [90–92] for special structured total least-squares problems with data matrix $C = [A \;\; b]$ that is Hankel or composed of a Hankel block A and an unstructured column b. They use the structured total least norm approach but recognize that a matrix appearing in the kernel subproblem of the algorithm has low displacement rank. This structure is exploited using the Schur algorithm.

The structured total least-squares solution methods outlined above point out the following issues:

- *Structure:* The structure specification for the data matrix C varies from general affine to specific affine, like Hankel/Toeplitz, or Hankel/Toeplitz block augmented with an unstructured column.
- *Rank reduction:* All methods, except for [87–89], reduce the rank of the data matrix by one.
- *Computational efficiency:* The efficiency varies from cubic for the methods that use a general affine structure to linear for the efficient methods of Lemmerling et al. [90] and Mastronardi et al. [91] that use a Hankel/Toeplitz type structure.

Efficient algorithms for problems with block-Hankel/Toeplitz structure and rank reduction with more than one are proposed by Markovsky et al. [93–95]. In addition, a numerically reliable and robust software implementation is available [96].

5.3. Structured total least-squares problem formulation and solution method

Let $\mathscr{S} : \mathbb{R}^{n_p} \to \mathbb{R}^{m\times(n+d)}$ be an injective function. A matrix $C \in \mathbb{R}^{m\times(n+d)}$ is said to be $\mathscr{S}$-structured if $C \in \text{image}(\mathscr{S})$. The vector p for which $C = \mathscr{S}(p)$ is called the parameter vector of the structured matrix C. Respectively, $\mathbb{R}^{n_p}$ is called the parameter space of the structure $\mathscr{S}$.

> The aim of the structured total least-squares problem is to perturb as little as possible a given parameter vector p by a vector Δp, so that the perturbed structured matrix $\mathscr{S}(p+\Delta p)$ becomes rank deficient with rank at most n.

Problem 14 (*Structured total least squares*). Given a data vector $p \in \mathbb{R}^{n_p}$, a structure specification $\mathscr{S} : \mathbb{R}^{n_p} \to \mathbb{R}^{m\times(n+d)}$, and a rank specification n, solve the optimization problem

$$\Delta p_{\text{stls}} = \arg\min_{\Delta p} \|\Delta p\| \quad \text{subject to } \operatorname{rank}(\mathscr{S}(p-\Delta p)) \leqslant n.$$

In what follows, we will use the input/output representation

$$\mathscr{S}(p-\Delta p)X_{\text{ext}} = 0, \quad X_{\text{ext}} := \begin{bmatrix} X \\ -I \end{bmatrix}$$

of the rank constraint, so that the structured total least-squares problem becomes the following parameter optimization problem

$$\widehat{X}_{\text{stls}} = \arg\min_{X,\Delta p} \|\Delta p\|$$

$$\text{subject to} \quad \mathscr{S}(p-\Delta p)\begin{bmatrix} X \\ -I \end{bmatrix} = 0. \qquad (\text{STLS}_{\text{X}})$$

The structured total least-squares problem is said to be affine structured if the function $\mathscr{S}$ is affine, i.e.,

$$\mathscr{S}(p) = S_0 + \sum_{i=1}^{n_p} S_i p_i \quad \text{for all } p \in \mathbb{R}^{n_p}$$

$$\text{and for some } S_i,\ i = 1,\ldots,n_p. \qquad (\text{AFF})$$

In an affine structured total least-squares problem, the constraint $\mathscr{S}(p-\Delta p)X_{\text{ext}} = 0$ is bilinear in the decision variables X and Δp.

Lemma 15. *Let* $\mathscr{S} : \mathbb{R}^{n_p} \to \mathbb{R}^{m\times(n+d)}$ *be an affine function. Then*

$$\mathscr{S}(p-\Delta p)X_{\text{ext}} = 0 \;\Leftrightarrow\; G(X)\Delta p = r(X),$$

where

$$G(X) := [\operatorname{vec}((S_1 X_{\text{ext}})^\top) \ \cdots \ \operatorname{vec}((S_{n_p} X_{\text{ext}})^\top)] \in \mathbb{R}^{md \times n_p}, \tag{G}$$

and

$$r(X) := \operatorname{vec}((\mathscr{S}(p) X_{\text{ext}})^\top) \in \mathbb{R}^{md}.$$

Using Lemma 15, we rewrite the affine structured total least-squares problem as follows:

$$\min_X \left(\min_{\Delta p} \|\Delta p\| \ \text{ subject to } \ G(X)\Delta p = r(X) \right). \tag{STLS$'_X$}$$

The inner minimization problem has an analytic solution, which allows to derive an equivalent optimization problem.

Theorem 16 (*Equivalent optimization problem for affine structured total least squares*). *Assuming that* $n_p \geqslant md$, *the affine structured total least squares problem* (STLS$_X$) *is equivalent to*

$$\min_X r^\top(X) \Gamma^\dagger(X) r(X) \quad \text{where } \Gamma(X) := G(X) G^\top(X), \tag{STLS$''_X$}$$

and $\Gamma^\dagger$ *is the pseudoinverse of* Γ.

The significance of Theorem 16 is that the constraint and the decision variable Δp in problem (STLS$_X$) are eliminated. Typically the number of elements nd in X is much smaller than the number of elements n_p in the correction Δp. Thus the reduction in the complexity is significant.

The equivalent optimization problem (SRLS$''_X$) is a nonlinear least-squares problem, so that classical optimization methods can be used for its solution. The optimization methods require a cost function and first derivative evaluation. In order to evaluate the cost function for a given value of the argument X, we need to form the weight matrix $\Gamma(X)$ and to solve the system of equations $\Gamma(X)y(X) = r(X)$. This straightforward implementation requires $O(m^3)$ floating point operation (flops). For large m (the applications that we aim at) this computational complexity becomes prohibitive.

It turns out, however, that for the special case of affine structures

$$\mathscr{S}(p) = [C^1 \ \ldots \ C^q] \quad \text{for all } p \in \mathbb{R}^{n_p}$$
$$\text{where } C^l, \text{ for } l = 1, \ldots, q, \text{ is}$$
$$\text{block-Toeplitz, block-Hankel,}$$
$$\text{unstructured, or exact.} \tag{A}$$

the weight matrix $\Gamma(X)$ has a block-Toeplitz and block-banded structure, which can be exploited for efficient cost function and first derivative evaluations. According to Assumption (A), $\mathscr{S}(p)$ is composed of blocks, each one of which is block-Toeplitz, block-Hankel, unstructured, or exact (an exact block C^l is not modified in the solution $\widehat{C} := \mathscr{S}(p - \Delta p)$, i.e., $\widehat{C}^l = C^l$).

Theorem 17 (*Structure of the weight matrix* Γ *[93]*). *Consider the equivalent optimization problem* (STLS$'_X$). *If in addition to the assumptions of Theorem* 16, *the structure* $\mathscr{S}$ *is such that* (A) *holds, then the weight matrix* $\Gamma(X)$ *has the block-Toeplitz and block-banded structure*:

$$\Gamma(X) = \begin{bmatrix} \mathbf{\Gamma}_0 & \mathbf{\Gamma}_1^\top & \cdots & \mathbf{\Gamma}_s^\top & & \mathbf{0} \\ \mathbf{\Gamma}_1 & \ddots & \ddots & \ddots & \ddots & \\ \vdots & \ddots & \ddots & \ddots & \ddots & \mathbf{\Gamma}_s^\top \\ \mathbf{\Gamma}_s & \ddots & \ddots & \ddots & \ddots & \vdots \\ & \ddots & \ddots & \ddots & \ddots & \mathbf{\Gamma}_1^\top \\ \mathbf{0} & & \mathbf{\Gamma}_s & \cdots & \mathbf{\Gamma}_1 & \mathbf{\Gamma}_0 \end{bmatrix},$$

where $s = \max_{l=1,\ldots,q}(\mathbf{n}_l - 1)$ and $\mathbf{n}_l$ *is the number of block columns in the block* C^l.

6. Conclusions

We reviewed the development and extensions of the classical total least-squares problem and presented a new total least-squares problem formulation. The new formulation is a matrix low rank approximation problem and allows for different representations of the rank constraint. Once a representation is fixed the matrix low rank approximation problem becomes a parameter optimization problem. The classical total least-squares formulation results from the new one when an input/output representation is chosen. The input/output representation is a linear system of equations $AX = B$, which is the classical way of addressing approximation problems. However, the input/output representation is not equivalent to the low rank constraint, which leads to non-generic total least-squares problems. Using the representation-free formulation, we classified existing total least-squares solution methods. The existing methods differ in the representation and the optimization method used.

The basic and generalized total least-squares problems have an analytic solution in terms of the singular value decomposition of the data matrix, which allows fast and reliable computation of the solution. Moreover, *all globally optimal solutions* can be classified in terms of the singular value decomposition. In contrast, more general total least-squares problems like the weighted and structured total least-squares problems require numerical optimization methods, which at best find a *single locally optimal solution*. The separation between the global total least-squares problem and general weighted and structured total least-squares problems is an important dividing line in the total least-squares hierarchy.

We emphasized the double minimization structure of the total least-squares problems and showed how it can be used for deriving efficient solution methods. The key step in our approach is the elimination of the correction by analytically minimizing over it. Then the structure of the data and weight matrices are exploited for efficient cost function and first derivative evaluation.

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