

## On the Equivalence of Constrained Total Least Squares and Structured Total Least Squares

Philippe Lemmerling, Bart De Moor, and Sabine Van Huffel

**Abstract**—Several extensions of the total least squares (TLS) method that are able to calculate a structured rank deficient approximation of a data matrix have been developed recently. The main result of this correspondence is the demonstration of the equivalence of two of these approaches, namely, the constrained total least squares (CTLS) approach and the structured total least squares (STLS) approach. We also present a numerical comparison of both methods.

### I. INTRODUCTION

The total least squares (TLS) approach for solving an overdetermined system  $Px \approx q$  is a very popular technique in linear parameter estimation problems. It can be formulated as follows:

$$\min_{\Delta P, \Delta q} \|[\Delta P \quad \Delta q]\|_F \text{ such that } q + \Delta q \in \text{Range}(P + \Delta P).$$

The standard procedure for solving this TLS problem involves the singular value decomposition (SVD) of the extended data matrix  $[P \quad q]$  [7]. However, the SVD does not preserve the structure of the extended data matrix  $[P \quad q]$ . This implies that the TLS approach will not yield the statistically optimal parameter vector  $x$  in the frequently occurring case where the extended data matrix is structured (Hankel, Toeplitz, sparse matrices, etc.).

Therefore, different approaches have been proposed, in which the structure of  $[P + \Delta P \quad q + \Delta q]$  can be made the same as the original structure of  $[P \quad q]$ . In order to do so, some methods, such as the constrained total least squares (CTLS) method, impose a structure on  $[\Delta P \quad \Delta q]$ , whereas other methods, such as the structured total least squares (STLS) method, impose a structure on  $[P + \Delta P \quad q + \Delta q]$ .

In this correspondence, we will focus on the CTLS [1], [2] and STLS [3], [4] approach. The structure of the correspondence is as follows. In Section II, we give a short overview of the formulation of the two approaches together with their solution methods. Section III contains the major contribution since it proves the equivalence of the CTLS and STLS approach under weak assumptions. Finally, in Section IV, we present a numerical example that illustrates the equivalence of both approaches. The convergence rate as well as the accuracy of the employed solution methods are briefly discussed. Further misleading arguments are dismissed and clarified.

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### II. PROBLEM FORMULATION

In this section, we briefly review the problem formulation of the CTLS and the STLS approaches as stated in [1] and in [4]. First, we introduce our notation. Let  $P, \Delta P \in \mathbb{R}^{m \times n}$ ,  $q, \Delta q \in \mathbb{R}^{m \times 1}$ . Let  $S = [P \quad q]$  and  $T = [P + \Delta P \quad q + \Delta q]$  where

- $M(:, i)$   $i$ th column of the matrix  $M$
- $M(i, :)$   $i$ th row of the matrix  $M$
- $M(i, j)$  entry on the  $i$ th row and in the  $j$ th column of the matrix  $M$
- $m(i)$   $i$ th component of the vector  $m$ .

#### A. CTLS

Let  $x \in \mathbb{R}^{n \times 1}$ ,  $F_i \in \mathbb{R}^{m \times k}$ ,  $i = 1, \dots, n+1$ ,  $f \in \mathbb{R}^{k \times 1}$ , and  $W \in \mathbb{R}^{k \times k}$ . The CTLS approach is the following:

$$\min_{f, x} f^t W f \text{ such that } (P + \Delta P)x = q + \Delta q, \quad (1)$$

in which  $W$  is a diagonal weighting matrix,  $\Delta P = [F_1 f \dots F_n f]$ , and  $\Delta q = F_{n+1} f$ . In this representation,  $f$  is a noise vector of sufficient and minimal dimension. By sufficient, we mean that the dimension must be high enough to describe the errors on the different columns. The structure of  $\Delta P$  and  $\Delta q$  can be imposed by choosing appropriate matrices  $F_i$ ,  $i = 1, \dots, n+1$ . In [1], it is proven, by using the method of Lagrange multipliers, that problem (1) can be solved by solving the optimization problem

$$\min_x [x^t \quad -1] S^t (H_x W^{-1} H_x^t)^{-1} S [x^t \quad -1]^t, \quad (2)$$

in which  $H_x = \sum_{i=1}^n x(i) F_i - F_{n+1}$ . The method we will use to optimize (2) is a quasi-Newton method using the BFGS rule for updating the Hessian [6].

#### B. STLS

Let  $S_i$ ,  $i = 0, \dots, k \in \mathbb{R}^{m \times (n+1)}$ ,  $t, s \in \mathbb{R}^{k \times 1}$ ,  $y \in \mathbb{R}^{(n+1) \times 1}$ , and  $W \in \mathbb{R}^{k \times k}$ , which is a diagonal weighting matrix. By taking  $k$  large enough and by choosing appropriate fixed matrices  $S_i$ , we can represent  $S$  by  $S_0 + \sum_{i=1}^k s(i) S_i$  and  $T$  by  $S_0 + \sum_{i=1}^k t(i) S_i$ . The STLS approach starts from the following formulation:

$$\min_{t, y} \sum_{i=1}^k W(i, i) [s(i) - t(i)]^2 \text{ such that } T y = 0, \quad y^t y = 1. \quad (3)$$

Observe that the structure of  $T$  is forced to be the same as the structure of  $S$  because we wrote  $T$  as an affine combination of the same  $S_i$  as we used for  $S$ .

In [4], the method of Lagrange multipliers is used to derive a problem that is equivalent to (3), namely, find the triplet  $(u, \tau, v)$  corresponding to the minimal  $\tau$  that satisfies

$$S v = D_v u \tau \quad u^t D_v u = 1 \quad (4)$$

$$S^t u = D_u v \tau \quad v^t D_u v = 1 \quad (5)$$

where  $D_u$  is defined via  $D_u v = \sum_{i=1}^k S_i^t (u^t S_i v) u$ , and likewise,  $D_v$  is defined via  $D_v u = \sum_{i=1}^k S_i (u^t S_i v) v$ . In [4], (4) and (5) are

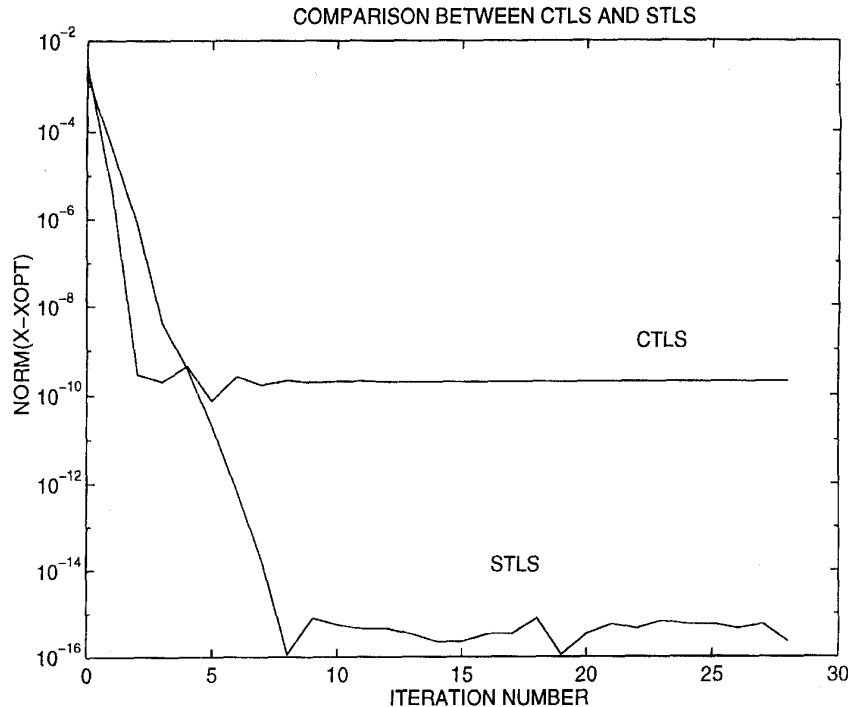


Fig. 1.  $\text{norm}(x - x_{opt})$  as a function of the iteration number. For the CTLS approach a quasi-Newton method is used with the BFGS rule for updating of the Hessian. The STLS approach uses an inverse iteration algorithm. The start value for  $x$  was  $x_{start} = 7.644999395502275e - 01$ . The example is the modeling example described in Section IV.

called the Riemannian SVD and are solved using an inverse iteration algorithm.

### III. PROOF OF EQUIVALENCE

The major result of this section is the equivalence of STLS and CTLS.

*Lemma 1:* Let  $A \in \mathbb{R}^{g \times h}$ ,  $y \in \mathbb{R}^{h \times 1}$ ,  $Q_y \in \mathbb{R}^{g \times g}$ , where the elements of  $Q_y$  are quadratic functions of the components of  $y$ . Let  $f$  be a multivariable function of  $y$ :  $f(y) = y^t A^t Q_y^{-1} A y$ . Then,  $f(\alpha y) = f(y)$ ,  $\forall \alpha \neq 0$ .

*Proof:* By the definition of  $f$ , we have  $f(\alpha y) = (\alpha y)^t A^t Q_{\alpha y}^{-1} A(\alpha y)$ . Since the elements of  $Q_{\alpha y}$  are quadratic functions of the components of  $\alpha y$ , we have  $Q_{\alpha y} = \alpha^2 Q_y$ . Therefore, we have  $f(\alpha y) = \alpha y^t A^t \alpha^{-2} Q_y^{-1} A y \alpha = y^t A^t Q_y^{-1} A y = f(y)$ ,  $\forall \alpha \neq 0$ .

*Proposition 1:* Let  $x_{opt} \in \mathbb{R}^{n \times 1}$  be the vector that solves the CTLS problem formulation (1), and let  $y_{opt} \in \mathbb{R}^{(n+1) \times 1}$  be a vector that solves the STLS problem formulation (3), without the regularization constraint  $y^t y = 1$ . If  $y_{opt}(n+1) \neq 0$  and  $D_y$  nonsingular, we can find an  $y_{opt}$  such that  $x_{opt} = y_{opt}(1:n)$  and  $y_{opt}(n+1) = -1$ , which proves the equivalence of the CTLS and STLS approach.

*Proof:* To prove this proposition, we will show that under the weak assumption  $y_{opt}(n+1) \neq 0$ , we can derive from the STLS formulation an objective function equal to the one in (2). This implies that both methods yield the same parameter vector, which proves their equivalence.

First, we write down the Lagrangian of the STLS problem formulation (3):

$$L(t, l, \lambda, y) = \sum_{i=1}^k W(i, i) [s(i) - t(i)]^2 - l^t T y - \lambda y^t y.$$

Putting  $\delta L / \delta l = 0$ ,  $\delta L / \delta y = 0$ ,  $\delta L / \delta t(i) = 0$ ,  $\forall i > 0$ , and  $\delta L / \delta \lambda = 0$ , we obtain

$$S y = D_y l \quad (6)$$

with

$$D_y = \sum_{i=1}^k \frac{1}{W(i, i)} (S_i y)(S_i y)^t \quad (7)$$

$$S^t l = D_y l$$

with

$$D_t = \sum_{i=1}^k \frac{1}{W(i, i)} (S_i^t l)(S_i^t l)^t$$

$$s(i) - t(i) = \frac{1}{W(i, i)} l^t S_i y, \quad \forall i > 0 \quad (8)$$

$$y^t y = 1. \quad (9)$$

Therefore, from (6), we obtain

$$l = D_y^{-1} S y \quad (10)$$

Using (7), (8), and (10), the STLS objective function becomes

$$\begin{aligned} \sum_{i=1}^k W(i, i) [s(i) - t(i)]^2 &= l^t \sum_{i=1}^k \frac{1}{W(i, i)} S_i (l^t S_i y) y \\ &= l^t D_y l \end{aligned} \quad (11)$$

$$= y^t S^t D_y^{-1} S y. \quad (12)$$

Let  $H_y = \sum_{i=1}^{n+1} y_i F_i$ . By using the latter definition, (7), and the fact that  $F_i = [S_1(:, i) S_2(:, i) \cdots S_k(:, i)]$ , it is straightforward to find that  $H_y W^{-1} H_y^t = D_y$ . Therefore, (12) becomes

$$y^t S^t (H_y W^{-1} H_y^t)^{-1} S y. \quad (13)$$

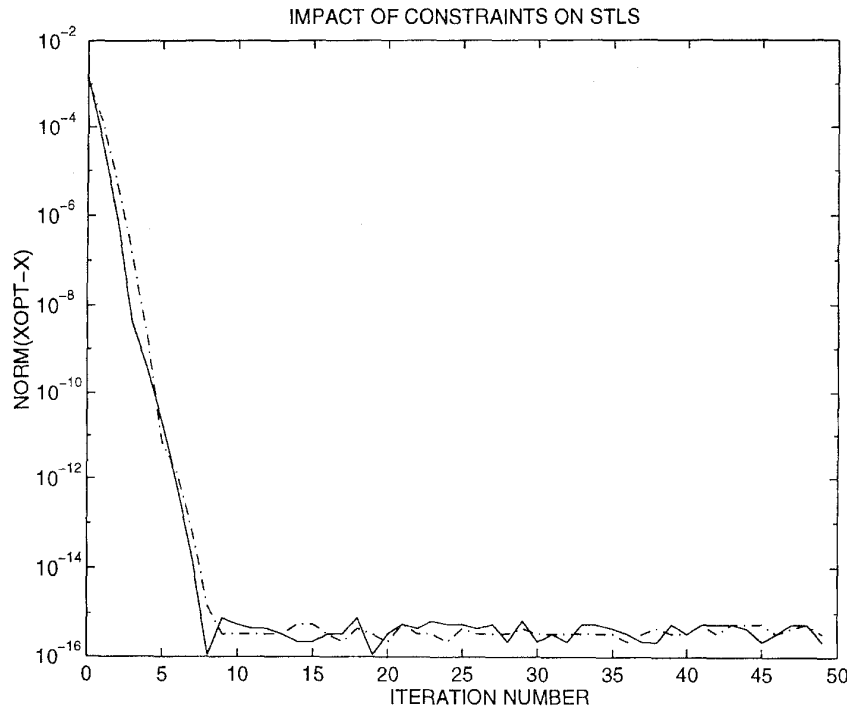


Fig. 2.  $\text{norm}(x-x_{opt})$  as a function of the iteration number for two different solution methods of the STLS approach. Both solution methods are inverse iteration algorithms, but the full line represents the case in which we use the constraint  $v^t v = 1$ , whereas the dotted line represents the case in which we use the constraint  $v^t D_u v = 1$ . The example is the modeling example described in Section IV.

If the condition  $y_{opt}(n+1) \neq 0$  is satisfied, we see that by applying Lemma 1 to (12),  $y(n+1)$  can be put equal to  $-1$  without affecting the solution of the STLS problem. If we put  $y(n+1) = -1$ , then  $H_y = H_x$ , and (13) becomes equal to (2). This means that the STLS objective function (13) is the same as the CTLS objective function (2). The latter implies that both objective functions will attain their minimum in the same parameter vector  $y(1:n) = x$ .  $\square$

#### IV. FURTHER COMMENTS

We use the example presented in [4]. In this example, we try to approximate a  $5 \times 2$  Toeplitz matrix by a rank deficient one which has the same structure. The advantage of this example is that we know the exact solution. We take the following example:

$$S = \begin{bmatrix} z_5 & z_4 & z_3 & z_2 & z_1 \\ z_6 & z_5 & z_4 & z_3 & z_2 \end{bmatrix}^t \\ = \begin{bmatrix} 2 & 3 & 4 & 5 & 6 \\ 1 & 2 & 3 & 4 & 5 \end{bmatrix}^t$$

which we will try to approximate by the best rank 1 structure-preserving approximation

$$\tilde{S} = \begin{bmatrix} \tilde{z}_5 & \tilde{z}_4 & \tilde{z}_3 & \tilde{z}_2 & \tilde{z}_1 \\ \tilde{z}_6 & \tilde{z}_5 & \tilde{z}_4 & \tilde{z}_3 & \tilde{z}_2 \end{bmatrix}^t$$

to  $S$  such that  $\sum_{i=1}^5 W(i, i)(\tilde{z}_i - z_i)^2$  is minimized, where the diagonal of  $W$  is  $[1 \ 2 \ 2 \ 2 \ 1]$ . In [4] and [8], the optimal  $x$  value (see (2) and (12); note that the  $y$  value in (12) that corresponds to the  $x$  value in (2) is  $y(1:n) = x$  and  $y(n+1) = -1$ )  $x_{opt}$  is calculated:  $x_{opt} = 0.7629230150743218$ . In the CTLS approach, we use the quasi-Newton method, with the BFGS rule for updating the Hessian to optimize (2). The STLS approach finds the solution to (4) and (5) by using an inverse iteration algorithm [4].

In Fig. 1, we see that both methods converge to the same value. As expected, the convergence rate of the inverse iteration algorithm is linear, whereas the quasi-Newton method has a faster super linear convergence rate. However, a lot of research still has to be done on algorithms for solving the CTLS or STLS problem. One of the interesting developments in this research area are the continuous time algorithms that have recently been developed for the Riemannian SVD [5].

In Fig. 1, we also see that the quasi-Newton algorithm is not as accurate as the inverse iteration algorithm. The reason for this inaccuracy can be found by comparing (2), (4), and (5). The accuracy in (2) is lost because of the "squaring effect" of  $S^t(H_x W^{-1} H_x^t)^{-1} S$ . In (4) and (5),  $S$  does not appear in such a product in which  $S^t$  and  $S$  are multiplied. In fact, this is the same reason why we would use an SVD of  $S$  and not the eigenvalue decomposition (EVD) of  $S^t S$  or  $S S^t$  if we want to calculate the singular values of  $S$ . Intuitively, it is very easy to see a connection between the EVD and the SVD on one hand and the CTLS and STLS method on the other hand. Clearly, the STLS kernel problem can be seen as a nonlinear SVD, with smallest singular value  $\tau$ . From (4), (5), and Lemma 1, we see that  $v$  can be found by minimizing  $v^t S^t D_v^{-1} S v = \tau^2$  with  $v^t \Xi v = 1$ ,  $\Xi$  being positive definite. In the latter, we clearly recognize the CTLS objective function, and we see that is very similar to an EVD in which we try to find the smallest eigenvalue  $\tau^2$ .

As opposed to earlier claims in [4] and [9], Lemma 1 clearly proves that  $\Xi$  can be any positive definite matrix. Fig. 2 illustrates this: We show the inverse iteration applied to (4) and (5) (dotted line) and the inverse iteration applied to (4) and (5) but with the  $v^t v = 1$  as the only constraint (full line).

Finally, we want to stress that solving (2) by applying an iterative eigenvalue decomposition (see [9]) to  $S^t(H_x W^{-1} H_x^t)^{-1} S$  is bound

to fail since this will lead to a stationary point  $x_{stat}$  that satisfies

$$S^t(H_{x_{stat}}W^{-1}H_{x_{stat}})^{-1}S[x_{stat} \ -1]^t = \lambda[x_{stat} \ -1]^t. \quad (14)$$

However, (14) is by no means a condition for optimality of (2).

## V. CONCLUSIONS

In this correspondence, we have proven the equivalence of the CTLS and the STLS approach. The equivalence was illustrated by a numerical example in which we also briefly discussed the convergence rate and the accuracy of the solution methods. Further misunderstandings have been clarified.

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## Estimation of the Parameters of a Random Amplitude Sinusoid by Correlation Fitting

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**Abstract**—In this correspondence, we consider the best asymptotic accuracy that can be achieved when estimating the parameters of a random-amplitude sinusoid from its sample covariances. An estimator based on matching in a weighted least-squares sense the sample correlation sequence to the theoretical sequence is presented. The asymptotic properties of the estimator are analyzed. A lower bound on the estimation of the parameters from sample covariances is derived. This bound is shown to be attainable by appropriately choosing the weighting matrix. However, the unweighted nonlinear least-squares estimate performance is shown to come close to the lower bound. The influence of the number of samples, the number of correlation samples, and the lowpass envelope characteristics are studied. Finally, a comparison with Yule–Walker (YW) methods is given.

## I. INTRODUCTION

In assessing the performance of any estimator of a parameter vector, it is of interest to establish the ultimate statistical performance that can be achieved in a given class of methods. The Cramér–Rao bound (CRB) [4], [6], [12] provides a lower bound on the covariance of any unbiased estimate of the parameter vector in question. However, in certain applications, it may be difficult to derive such a bound. Furthermore, it is often of primary concern to calculate lower bounds for estimators in a certain class. For instance, in the case of ARMA or sinusoids-in-noise processes, most high-resolution methods, such as high-order Yule–Walker (YW) [10], MUSIC [8], and ESPRIT [7] rely on the sample covariances of the process considered. Consequently, the following question naturally arises: What is the best accuracy that can be achieved by processing the sample covariances? This question has been addressed for the case of ARMA processes in [5], [6], and [9] and for sinusoids-in-noise signals in [11].

In this correspondence, we are interested in the best consistent estimation of the parameters of a random-amplitude sinusoidal signal from its sample covariances. For this type of application, derivation of the CRB is an open problem (see, however, [3] for related work). The objective of this work is threefold. First, we show how an asymptotically best consistent (ABC) estimate of the parameters can be obtained from sample covariances. We derive an algorithm based on matching, in a weighted least squares sense, a sequence of sample correlations to their theoretical values. The asymptotic covariance matrix of the estimation errors is derived. Second, we derive the lower bound on the covariance matrix of any estimator based on a finite number of sample correlations. It is shown that this bound can be attained by an appropriate choice of the weighting matrix in the correlation matching algorithm. The bound derived herein is believed to be of interest since it is a reference against which numerous methods could be compared. Third, we propose to use the *unweighted* least-squares estimator, which we call the nonlinear

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