SIAM J. MATRIX ANAL. APPL.
Vol. 26, No. 4, pp. 1083–1099 

# BLOCK-TOEPLITZ/HANKEL STRUCTURED TOTAL LEAST SQUARES*

IVAN MARKOVSKY†, SABINE VAN HUFFEL†, AND RIK PINTELON‡

**Abstract.** A structured total least squares problem is considered in which the extended data matrix is partitioned into blocks and each of the blocks is block-Toeplitz/Hankel structured, unstructured, or exact. An equivalent optimization problem is derived and its properties are established. The special structure of the equivalent problem enables us to improve the computational efficiency of the numerical solution methods. By exploiting the structure, the computational complexity of the algorithms (local optimization methods) per iteration is linear in the sample size. Application of the method for system identification and for model reduction is illustrated by simulation examples.

**Key words.** parameter estimation, total least squares, structured total least squares, system identification, model reduction

**AMS subject classifications.** 15A06, 62J12, 37M10

**DOI.** 10.1137/S0895479803434902

## 1. Introduction.

The *total least squares* (TLS) problem

$$\min_{\Delta A, \Delta B, X} \left\| \begin{bmatrix} \Delta A & \Delta B \end{bmatrix} \right\|_{\mathrm{F}}^2 \quad \text{subject to} \quad (A - \Delta A)X = B - \Delta B, \tag{1.1}$$

where $A \in \mathbb{R}^{m \times n}$, $B \in \mathbb{R}^{m \times d}$, $C := [A \ B]$ is the data matrix, and $X \in \mathbb{R}^{n \times d}$ is the parameter of interest, proved to be a useful parameter estimation technique. It became especially popular since the early eighties due to the development [8] of reliable solution methods based on singular value decomposition. The same technique is known in the system identification literature as the Koopmans–Levin method [12] and in the statistical literature as orthogonal regression [7]. For a comprehensive introduction to the theory, algorithms, and applications of the TLS method, see [25].

With the increased interest in the TLS technique, more and more researchers started to apply it in various applications. In some cases, however, important assumptions of the method are not satisfied, which resulted in the development of appropriate extensions of the original TLS method. We mention the *mixed LS-TLS method*

*Received by the editors September 15, 2003; accepted for publication (in revised form) by L. Eldén June 30, 2004; published electronically May 6, 2005. This research was supported by Research Council K. U. Leuven through grants GOA-Mefisto 666, IDO/99/003, and IDO/02/009 (predictive computer models for medical classification problems using patient data and expert knowledge) and several Ph.D./postdoctorate and fellow grants; the Flemish Government, FWO, through Ph.D./postdoctorate grants, projects, and grants G.0200.00 (damage detection in composites by optical fibers), G.0078.01 (structured matrices), G.0407.02 (support vector machines), G.0269.02 (magnetic resonance spectroscopic imaging), and G.0270.02 (nonlinear Lp approximation); research communities (ICCoS, ANMMM); the AWI under the Bil. Int. Collaboration Hungary/Poland; the IWT through Ph.D. grants; the Belgian Federal Government, DWTC (grants IUAP IV-02 (1996–2001) and IUAP V-22 (2002–2006): Dynamical Systems and Control: Computation, Identification & Modelling); the EU through NICONET, INTERPRET, PDT-COIL, MRS/MRI signal processing (TMR); and contract research/agreements (Data4s, IPCOS).

http://www.siam.org/journals/simax/26-4/43490.html

†ESAT-SCD (SISTA), Katholieke Universiteit Leuven, Kasteelpark Arenberg 10, B-3001 Leuven-Heverlee, Belgium (Ivan.Markovsky@esat.kuleuven.ac.be, Sabine.VanHuffel@esat.kuleuven.ac.be). The first author was supported by a K.U. Leuven doctoral scholarship.

‡Department ELEC, Vrije Universiteit Brussel, Pleinlaan 2, B-1050 Brussels, Belgium (Rik.Pintelon@vub.ac.be).

[25, sect. 3.5], where some of the columns of $A$ are exact (noise free), and the so-called *generalized total least squares method* [24], where the cost function of TLS problem (1.1) is generalized to $\| \begin{bmatrix} \Delta A & \Delta B \end{bmatrix} V \|_{\mathrm{F}}^2$, with $V \geq 0$. The latest developments in the field are collected in the proceedings books [22, 23].

In the early nineties, a powerful generalization of the TLS method was put forward [1, 4, 20]. The so-called *structured total least squares* (STLS) problem,

$$\min_{\Delta A, \Delta B, X} \left\| \begin{bmatrix} \Delta A & \Delta B \end{bmatrix} \right\|_{\mathrm{F}}^2 \quad \text{subject to} \quad (A - \Delta A)X = B - \Delta B \quad \text{and}$$
$$\begin{bmatrix} \Delta A & \Delta B \end{bmatrix} \text{ has the same structure as } \begin{bmatrix} A & B \end{bmatrix},$$

defined in the same way as the TLS problem (1.1) but with the additional structure constraint, includes as special cases many of the presently known TLS variations. The structure occurs naturally in, e.g., applications dealing with discrete-time dynamic phenomena [6], where the Hankel and Toeplitz matrices are fundamental.

Although the STLS problem is very general, it is still not widely accepted due to the lack of reliable solution methods for its computation, the main difficulty being that, as an optimization problem, it is nonconvex and there is no guarantee that a global minimum point will be found. Still, under certain conditions [10] for highly overdetermined systems ($m \ll nd$) the solution of the problem is unique and the main difficulty—the presence of multiple local minima—tends to disappear for large sample sizes (i.e., for $m \to \infty$). In addition, due to the consistency results of [10], such an assumption guarantees accurate estimation and makes the problem meaningful from a statistical point of view.

However, the currently used numerical algorithms for solving the STLS problem can hardly deal with large sample sizes. The original methods of [1, 4, 20] have computational costs that increase quadratically or even cubically as a function of $m$. In [11, 17], methods with computational cost linear in $m$ are developed using the generalized Schur algorithm. These methods, however, are developed for a particular structure of the data matrix $C$ (in [11] $C$ is Hankel, and in [17] $A \in \mathbb{R}^{m \times n}$ is Toeplitz and $B \in \mathbb{R}^{m \times 1}$ is unstructured) and modifications for other structures are nontrivial.

In [13], based on the insight from [10], we have proposed a new approach with computational cost linear in $m$ and dealing with a flexible structure specification. The data matrix $C$ can be partitioned into blocks $C = \begin{bmatrix} C^{(1)} & \cdots & C^{(q)} \end{bmatrix}$, where each of the blocks $C^{(l)}$, for $l = 1, \dots, q$, is Hankel, Toeplitz, unstructured, or exact.

In this paper, we consider an extension of the results of [13] to the case of block-Hankel and block-Toeplitz structured matrices. Thus the data matrix is now a block matrix, of which the blocks are themselves structured with one of the four possible structures: block-Hankel, block-Toeplitz, unstructured, or exact. The need for such an extension comes from applications dealing with multi-input and/or multi-output dynamical systems. The proposed algorithms are implemented in C (see [15]), and the software is available.

Standard notation used in the paper is as follows: $\mathbb{R}$ for the set of the real numbers, $\mathbb{N}$ for the set of the natural numbers, $\|\cdot\|$ for the Euclidean norm, and $\|\cdot\|_{\mathrm{F}}$ for the Frobenius norm. The operator that vectorizes columnwise a matrix is denoted by $\mathrm{vec}(\cdot)$, the expectation operator by $\mathbf{E}$, and the covariance matrix of a random vector by $\mathrm{cov}(\cdot)$. The pseudoinverse of a matrix $A$ is denoted by $A^{\dagger}$.

**2. The STLS problem.** In this section, we define the STLS problem, considered in the paper, and derive an equivalent optimization problem. Consider a function $\mathcal{S} : \mathbb{R}^{n_p} \to \mathbb{R}^{m \times (n+d)}$ that defines the structure of the data as follows: a matrix $C \in \mathbb{R}^{m \times (n+d)}$ is said to have the structure defined by $\mathcal{S}$ if there exists a $p \in \mathbb{R}^{n_p}$, such that $C = \mathcal{S}(p)$. The vector $p$ is called a *parameter vector* for the structured matrix $C$.

PROBLEM 2.1 (STLS problem). *Given a data vector $p \in \mathbb{R}^{n_p}$ and a structure specification $\mathcal{S} : \mathbb{R}^{n_p} \to \mathbb{R}^{m\times(n+d)}$, solve the optimization problem*

$$\min_{X,\Delta p} \|\Delta p\|^2 \quad \text{subject to} \quad \mathcal{S}(p-\Delta p)\begin{bmatrix} X \\ -I_d \end{bmatrix} = 0. \tag{2.1}$$

The interpretation of (2.1) is the following: Find the smallest correction $\Delta p$, measured in 2-norm, that makes the structured matrix $\mathcal{S}(p-\Delta p)$ rank deficient with rank at most $n$. Define

$$X_{\text{ext}} := \begin{bmatrix} X \\ -I_d \end{bmatrix}, \quad \text{and} \quad \begin{bmatrix} A & B \end{bmatrix} := C := \mathcal{S}(p), \text{ where } A \in \mathbb{R}^{m\times n} \text{ and } B \in \mathbb{R}^{m\times d}.$$

$CX_{\text{ext}} = 0$ is shorthand notation for the structured system of equations $AX = B$.

The STLS problem is said to be *affine structured* if the function $\mathcal{S}$ is affine, i.e.,

$$\mathcal{S}(p) = S_0 + \sum_{i=1}^{n_p} S_i p_i \quad \text{for all } p \in \mathbb{R}^{n_p} \text{ and for some } S_i,\ i = 1,\dots,n_p. \tag{2.2}$$

In an affine STLS problem, the constraint $\mathcal{S}(p-\Delta p)X_{\text{ext}} = 0$ becomes bilinear in the decision variables $X$ and $\Delta p$.

LEMMA 2.2. *Let $\mathcal{S} : \mathbb{R}^{n_p} \to \mathbb{R}^{m\times(n+d)}$ be an affine function. Then*

$$\mathcal{S}(p-\Delta p)X_{ext} = 0 \iff G(X)\Delta p = r(X),$$

*where*

$$G(X) := \begin{bmatrix} \operatorname{vec}\big((S_1 X_{ext})^\top\big) & \cdots & \operatorname{vec}\big((S_{n_p} X_{ext})^\top\big) \end{bmatrix} \in \mathbb{R}^{md\times n_p} \tag{2.3}$$

*and*

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

*Proof.*

$$\begin{aligned} \mathcal{S}(p-\Delta p)X_{\text{ext}} = 0 &\iff \sum_{i=1}^{n_p} S_i \Delta p_i X_{\text{ext}} = \mathcal{S}(p)X_{\text{ext}} \\ &\iff \sum_{i=1}^{n_p} \operatorname{vec}\big((S_i X_{\text{ext}})^\top\big)\Delta p_i = \operatorname{vec}\Big(\big(\mathcal{S}(p)X_{\text{ext}}\big)^\top\Big) \\ &\iff G(X)\Delta p = r(X). \qquad \square \end{aligned}$$

Using Lemma 2.2, we rewrite the affine STLS problem as follows:

$$\min_X \Big( \min_{\Delta p} \|\Delta p\|^2 \quad \text{subject to} \quad G(X)\Delta p = r(X) \Big). \tag{2.4}$$

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

THEOREM 2.3 (equivalent optimization problem for affine STLS). *Assuming that $n_p \geq md$, the affine STLS problem* (2.4) *is equivalent to*

$$\min_X f_0(X), \text{ where } f_0(X) := r^\top(X)\Gamma^\dagger(X)r(X) \quad \text{and} \quad \Gamma(X) := G(X)G^\top(X). \tag{2.5}$$

*Proof.* Under the assumption $n_p \geq md$, the inner minimization problem of (2.4) is a least norm problem. Its minimum point (as a function of $X$) is

$$\Delta p_{\min}(X) = G^\top(X)\big(G(X)G^\top(X)\big)^\dagger r(X),$$

so that

$$f_0(X) = \Delta p_{\min}^\top(X)\Delta p_{\min}(X) = r^\top(X)\big(G(X)G^\top(X)\big)^\dagger r(X) = r^\top(X)\Gamma^\dagger(X)r(X). \qquad \square$$

The significance of Theorem 2.3 is that the constraint and the decision variable $\Delta p$ in problem (2.4) are eliminated. Note that typically the number of elements $nd$ in $X$ is much smaller than the number of elements $n_p$ in the correction $\Delta p$. Thus the reduction in the complexity is significant.

The equivalent optimization problem (2.5) 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 $f_0$ 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 a special case of affine structures $\mathcal{S}$, the weight matrix $\Gamma(X)$ is nonsingular and has a block-Toeplitz and block-banded structure, which can be exploited for efficient cost function and first derivative evaluations. The set of structures of $\mathcal{S}$, for which we establish the special properties of $\Gamma(X)$, is

$$\mathcal{S}(p) = \begin{bmatrix} C^{(1)} & \cdots & C^{(q)} \end{bmatrix} \text{ for all } p \in \mathbb{R}^{n_p}, \text{ where } C^{(l)}, \text{ for } l = 1, \ldots, q, \text{ is} \tag{2.6}$$
$$\text{block-Toeplitz, block-Hankel, exact, or unstructured}$$
$$\text{and all block-Toeplitz/Hankel structured blocks } C^{(l)}$$
$$\text{have equal row dimension } K \text{ of the blocks.}$$

Assumption (2.6) says that $\mathcal{S}(p)$ is composed of blocks, each of which is block-Toeplitz, block-Hankel, exact, or unstructured. A block $C^{(l)}$ that is exact is not modified in the solution $\hat{C} := \mathcal{S}(p - \Delta p)$, i.e., $\hat{C}^{(l)} = C^{(l)}$. Assumption 2.6 is the essential structural assumption that we impose on problem (2.1). As shown in section 6, it is fairly general and covers many applications.

*Example* 1. Consider the block-Toeplitz matrix

$$C = \begin{bmatrix} \boxed{\begin{matrix}5\\6\end{matrix}} & \boxed{\begin{matrix}3\\4\end{matrix}} & \boxed{\begin{matrix}1\\2\end{matrix}} \\ \boxed{\begin{matrix}7\\8\end{matrix}} & \boxed{\begin{matrix}5\\6\end{matrix}} & \boxed{\begin{matrix}3\\4\end{matrix}} \\ \boxed{\begin{matrix}9\\10\end{matrix}} & \boxed{\begin{matrix}7\\8\end{matrix}} & \boxed{\begin{matrix}5\\6\end{matrix}} \end{bmatrix}$$

with row dimension of the block $K = 2$. Next we specify the matrices $S_i$ that define via (2.2) an affine function $\mathcal{S}$, such that $C = \mathcal{S}(p)$ for a certain parameter vector $p$. Let $==$ be an elementwise comparison operator. Acting on matrices of the same size, it gives as a result a matrix with the same size as the arguments, of which the $(i,j)$th element is 1 if the corresponding elements of the arguments are equal, and 0 otherwise. (Think of MATLAB's $==$ operator.) Let $E$ be the $6 \times 3$ matrix with all elements equal to 1 and define $S_0 := 0_{6\times 3}$ and $S_i := (C == iE)$ for $i = 1, \ldots, 10$. We have

$$C = \sum_{i=1}^{10} S_i i = S_0 + \sum_{i=1}^{10} S_i p_i =: \mathcal{S}(p), \qquad \text{with } p = \begin{bmatrix} 1 & 2 & \cdots & 10 \end{bmatrix}^\top.$$

The matrix $C$ considered in the example is special; it allowed us to easily write down a corresponding affine function $\mathcal{S}$. Clearly with the constructed $\mathcal{S}$, *any* $6 \times 3$ block-Toeplitz matrix $C$ with row dimension of the block $K = 2$ can be written as $C = \mathcal{S}(p)$ for certain $p \in \mathbb{R}^{10}$.

We will use the notation $\mathbf{n}_l$ for the number of *block* columns of the block $C^{(l)}$. For unstructured and exact blocks, $\mathbf{n}_l := 1$.

**3. Properties of the weight matrix $\boldsymbol{\Gamma}$.** For the evaluation of the cost function $f_0$ of the equivalent optimization problem (2.5), we have to solve the system of equations $\Gamma(X)y(X) = r(X)$, where $\Gamma(X) \in \mathbb{R}^{md\times n_p}$ with both $m$ and $n_p$ large. In this section, we investigate the structure of the matrix $\Gamma(X)$. Occasionally we drop the explicit dependence of $r$ and $\Gamma$ on $X$.

THEOREM 3.1 (structure of the weight matrix $\Gamma$). *Consider the equivalent optimization problem* (2.5) *from Theorem* 2.3. *If, in addition to the assumptions of Theorem* 2.3, *the structure $\mathcal{S}$ is such that* (2.6) *holds, then the weight matrix $\Gamma(X)$ has the block-banded Toeplitz structure*

$$\Gamma(X) = \begin{bmatrix} \Gamma_0 & \Gamma_1^\top & \cdots & \Gamma_s^\top & & \mathbf{0} \\ \Gamma_1 & \ddots & \ddots & \ddots & \ddots & \\ \vdots & \ddots & \ddots & \ddots & \ddots & \Gamma_s^\top \\ \Gamma_s & \ddots & \ddots & \ddots & \ddots & \vdots \\ & \ddots & \ddots & \ddots & \ddots & \Gamma_1^\top \\ \mathbf{0} & & \Gamma_s & \cdots & \Gamma_1 & \Gamma_0 \end{bmatrix} \in \mathbb{R}^{md\times md}, \tag{3.1}$$

*where $\Gamma_k \in \mathbb{R}^{dK\times dK}$, for $k = 0, 1, \ldots, s$, and $s = \max_{l=1,\ldots,q}(\mathbf{n}_l - 1)$, where $\mathbf{n}_l$ is the number of block columns in the block $C^{(l)}$ of the data matrix $\mathcal{S}(p)$.*

The proof is developed in a series of lemmas. First we reduce the original problem with multiple blocks $C^{(l)}$ (see (2.6)) to three independent problems—one for the unstructured case, one for the block-Hankel case, and one for the block-Toeplitz case.

LEMMA 3.2. *Consider a structure specification of the form*

$$\mathcal{S}(p) = \begin{bmatrix} \mathcal{S}^{(1)}(p^{(1)}) & \cdots & \mathcal{S}^{(q)}(p^{(q)}) \end{bmatrix}, \qquad p^{(l)} \in \mathbb{R}^{n_p^{(l)}}, \quad \sum_{l=1}^{q} n_p^{(l)} =: n_p,$$

*where $p^\top =: \begin{bmatrix} p^{(1)\top} & \cdots & p^{(q)\top} \end{bmatrix}$ and $\mathcal{S}(p^{(l)}) := S_0^{(l)} + \sum_{i=1}^{n_p^{(l)}} S_i^{(l)} p_i^{(l)}$ for all $p^{(l)} \in \mathbb{R}^{n_p^{(l)}}$,*

$l = 1, \dots, q$. *Then*

$$\Gamma(X) = \sum_{l=1}^{q} \Gamma^{(l)}(X), \tag{3.2}$$

*where* $\Gamma^{(l)} := G^{(l)} G^{(l)\top}$, $G^{(l)} := [\mathrm{vec}((S_1^{(l)} X_{ext}^{(l)})^\top) \quad \cdots \quad \mathrm{vec}((S_{n_p^{(l)}}^{(l)} X_{ext}^{(l)})^\top)]$, *and*

$$X_{ext} =: \begin{bmatrix} X_{ext}^{(1)} \\ \vdots \\ X_{ext}^{(q)} \end{bmatrix}, \quad \textit{with} \quad X_{ext}^{(l)} \in \mathbb{R}^{n_l \times d}, \quad n_l := \mathrm{coldim}(C^{(l)}), \quad \sum_{l=1}^{q} n_l = n + d.$$

*Proof.* The result is a refinement of Lemma 2.2. Let $\Delta p^\top =: \left[\Delta p^{(1)\top} \ \cdots \ \Delta p^{(q)\top}\right]$, where $\Delta p^{(l)} \in \mathbb{R}^{n_p^{(l)}}$ for $l = 1, \dots, q$. We have

$$\begin{aligned} \mathcal{S}(p - \Delta p) X_{\mathrm{ext}} = 0 \iff & \sum_{l=1}^{q} \mathcal{S}^{(l)}(p^{(l)} - \Delta p^{(l)}) X_{\mathrm{ext}}^{(l)} = 0 \\ \iff & \sum_{l=1}^{q} \sum_{i=1}^{n_p} S_i^{(l)} \Delta p_i^{(l)} X_{\mathrm{ext}}^{(l)} = \mathcal{S}(p) X_{\mathrm{ext}} \\ \iff & \sum_{l=1}^{q} G^{(l)} \Delta p^{(l)} = r(X) \\ \iff & \underbrace{\begin{bmatrix} G^{(1)} & \cdots & G^{(q)} \end{bmatrix}}_{G(X)} \Delta p = r(X), \end{aligned}$$

so that $\Gamma = GG^\top = \sum_{l=1}^{q} G^{(l)} G^{(l)\top} = \sum_{l=1}^{q} \Gamma^{(l)}$. ∎

Next we establish the structure of $\Gamma$ for an STLS problem with an unstructured data matrix.

LEMMA 3.3. *Let*

$$\mathcal{S}(p) := \begin{bmatrix} p_1 & p_2 & \cdots & p_{n+d} \\ p_{n+d+1} & p_{n+d+2} & \cdots & p_{2(n+d)} \\ \vdots & \vdots & & \vdots \\ p_{(m-1)(n+d)+1} & p_{(m-1)(n+d)+2} & \cdots & p_{m(n+d)} \end{bmatrix} \in \mathbb{R}^{m \times (n+d)};$$

*then*

$$\Gamma = I_m \otimes (X_{ext}^\top X_{ext}); \tag{3.3}$$

*i.e., the matrix* $\Gamma$ *has the structure* (3.1) *with* $s = 0$ *and* $\Gamma_0 = I_K \otimes (X_{ext}^\top X_{ext})$.

*Proof.* We have

$$\begin{aligned} \mathcal{S}(p - \Delta p) X_{\mathrm{ext}} = 0 \iff & \mathrm{vec}\big(X_{\mathrm{ext}}^\top \mathcal{S}^\top(\Delta p)\big) = \mathrm{vec}\big((\mathcal{S}(p) X_{\mathrm{ext}})^\top\big) \\ \iff & \underbrace{(I_m \otimes X_{\mathrm{ext}}^\top)}_{G(X)} \underbrace{\mathrm{vec}\big(\mathcal{S}^\top(\Delta p)\big)}_{\Delta p} = r(X). \end{aligned}$$

Therefore, $\Gamma = GG^\top = (I_m \otimes X_{\mathrm{ext}}^\top)(I_m \otimes X_{\mathrm{ext}}^\top)^\top = I_m \otimes (X_{\mathrm{ext}}^\top X_{\mathrm{ext}})$. ∎

Next we establish the structure of $\Gamma$ for an STLS problem with a block-Hankel data matrix.

LEMMA 3.4. *Let*

$$\mathcal{S}(p) := \begin{bmatrix} C_1 & C_2 & \cdots & C_{\mathbf{n}} \\ C_2 & C_3 & \cdots & C_{\mathbf{n}+1} \\ \vdots & \vdots & & \vdots \\ C_{\mathbf{m}} & C_{\mathbf{m}+1} & \cdots & C_{\mathbf{m}+\mathbf{n}-1} \end{bmatrix} \in \mathbb{R}^{m\times(n+d)}, \qquad \mathbf{n} := \frac{n+d}{L}, \quad \mathbf{m} := \frac{m}{K},$$

*where $C_i$ are $K \times L$ unstructured blocks, parameterized by $p^{(i)} \in \mathbb{R}^{KL}$ as follows:*

$$C_i := \begin{bmatrix} p_1^{(i)} & p_2^{(i)} & \cdots & p_L^{(i)} \\ p_{L+1}^{(i)} & p_{L+2}^{(i)} & \cdots & p_{2L}^{(i)} \\ \vdots & \vdots & & \vdots \\ p_{(K-1)L+1}^{(i)} & p_{(K-1)L+2}^{(i)} & \cdots & p_{KL}^{(i)} \end{bmatrix} \in \mathbb{R}^{K\times L}.$$

*Define a partitioning of $X_{ext}$ as follows: $X_{ext}^\top =: \begin{bmatrix} X_1 & \cdots & X_{\mathbf{n}} \end{bmatrix}$, where $X_j \in \mathbb{R}^{d\times L}$. Then $\Gamma$ has the block-banded Toeplitz structure* (3.1) *with $s = \mathbf{n} - 1$ and with*

$$\Gamma_k = \sum_{j=1}^{\mathbf{n}-k} \mathbf{X}_j \mathbf{X}_{j+k}^\top, \quad \text{where} \quad \mathbf{X}_k := I_K \otimes X_k. \tag{3.4}$$

*Proof.* Define the residual $R := \mathcal{S}(\Delta p)X_{\text{ext}}$ and the partitioning $R^\top =: \begin{bmatrix} R_1 \cdots R_{\mathbf{m}} \end{bmatrix}$, where $R_1 \in \mathbb{R}^{d\times K}$. Let $\Delta C := \mathcal{S}(\Delta p)$, with blocks $\Delta C_i$. We have

$$\begin{aligned} &\mathcal{S}(p - \Delta p)X_{\text{ext}} = 0 \iff \mathcal{S}(\Delta p)X_{\text{ext}} = \mathcal{S}(p)X_{\text{ext}} \\ &\iff \begin{bmatrix} X_1 & X_2 & \cdots & X_{\mathbf{n}} & & & \\ & X_1 & X_2 & \cdots & X_{\mathbf{n}} & & \\ & & \ddots & \ddots & & \ddots & \\ & & & X_1 & X_2 & \cdots & X_{\mathbf{n}} \end{bmatrix} \begin{bmatrix} \Delta C_1^\top \\ \Delta C_2^\top \\ \vdots \\ \Delta C_{\mathbf{m}+\mathbf{n}-1}^\top \end{bmatrix} = \begin{bmatrix} R_1^\top \\ R_2^\top \\ \vdots \\ R_{\mathbf{m}}^\top \end{bmatrix} \\ &\iff \underbrace{\begin{bmatrix} \mathbf{X}_1 & \mathbf{X}_2 & \cdots & \mathbf{X}_{\mathbf{n}} & & & \\ & \mathbf{X}_1 & \mathbf{X}_2 & \cdots & \mathbf{X}_{\mathbf{n}} & & \\ & & \ddots & \ddots & & \ddots & \\ & & & \mathbf{X}_1 & \mathbf{X}_2 & \cdots & \mathbf{X}_{\mathbf{n}} \end{bmatrix}}_{G(X)} \underbrace{\begin{bmatrix} \text{vec}(\Delta C_1^\top) \\ \text{vec}(\Delta C_2^\top) \\ \vdots \\ \text{vec}(\Delta C_{\mathbf{m}+\mathbf{n}-1}^\top) \end{bmatrix}}_{\Delta p} = \underbrace{\begin{bmatrix} \text{vec}(R_1^\top) \\ \text{vec}(R_2^\top) \\ \vdots \\ \text{vec}(R_{\mathbf{m}}^\top) \end{bmatrix}}_{r(X)}. \end{aligned}$$

Therefore, $\Gamma = GG^\top$ has the structure (3.1), with $\Gamma_k$'s given by (3.4). ∎

The derivation of the $\Gamma$ matrix for an STLS problem with block-Toeplitz data matrix is analogous to the one for an STLS problem with block-Hankel data matrix. We state the result in the next lemma.

LEMMA 3.5. *Let*

$$\mathcal{S}(p) := \begin{bmatrix} C_{\mathbf{n}} & C_{\mathbf{n}-1} & \cdots & C_1 \\ C_{\mathbf{n}+1} & C_{\mathbf{n}} & \cdots & C_2 \\ \vdots & \vdots & & \vdots \\ C_{\mathbf{m}+\mathbf{n}-1} & C_{\mathbf{m}+\mathbf{n}-2} & \cdots & C_{\mathbf{m}} \end{bmatrix} \in \mathbb{R}^{m\times(n+d)},$$

*with the blocks $C_i$ defined as in Lemma* 3.4. *Then* $\Gamma$ *has the block-banded Toeplitz structure* (3.1) *with* $s = \mathbf{n} - 1$ *and with*

$$\Gamma_k = \sum_{j=k+1}^{\mathbf{n}} \mathbf{X}_j \mathbf{X}_{j-k}^\top. \tag{3.5}$$

*Proof.* Following the same derivation as in the proof of Lemma 3.4, we find that

$$G = \begin{bmatrix} \mathbf{X}_\mathbf{n} & \mathbf{X}_{\mathbf{n}-1} & \cdots & \mathbf{X}_1 & & & \\ & \mathbf{X}_\mathbf{n} & \mathbf{X}_{\mathbf{n}-1} & \cdots & \mathbf{X}_1 & & \\ & & \ddots & \ddots & & \ddots & \\ & & & \mathbf{X}_\mathbf{n} & \mathbf{X}_{\mathbf{n}-1} & \cdots & \mathbf{X}_1 \end{bmatrix}.$$

Therefore, $\Gamma = GG^\top$ has the structure (3.1), with $\Gamma_k$'s given by (3.5). ∎

*Proof of Theorem* 3.1. Lemmas 3.2–3.5 show that the weight matrix $\Gamma$ for the original problem has the block-banded Toeplitz structure (3.1) with $s = \max_{l=1,\dots,q}(\mathbf{n}_l - 1)$, where $\mathbf{n}_l$ is the number of block columns in the $l$th block of the data matrix. ∎

Apart from revealing the structure of $\Gamma$, the proof of Theorem 3.1 gives an algorithm for the construction of the blocks $\Gamma_0, \dots, \Gamma_s$ that define $\Gamma$:

$$\Gamma_k = \sum_{l=1}^{q} \Gamma_k^{(l)}, \text{ where } \Gamma_k^{(l)} = \begin{cases} \sum_{j=k+1}^{\mathbf{n}_l} \mathbf{X}_j^{(l)} \mathbf{X}_{j-k}^{(l)\top} & \text{if } C^{(l)} \text{ is block-Toeplitz,} \\ \sum_{j=1}^{\mathbf{n}_l - k} \mathbf{X}_j^{(l)} \mathbf{X}_{j+k}^{(l)\top} & \text{if } C^{(l)} \text{ is block-Hankel,} \\ 0_{dK} & \text{if } C^{(l)} \text{ is exact, or} \\ \delta_k I_K \otimes (X_{\text{ext}}^{(l)\top} X_{\text{ext}}^{(l)}) & \text{if } C^{(l)} \text{ is unstructured,} \end{cases} \tag{3.6}$$

where $\delta$ is the Kronecker delta function: $\delta_0 = 1$ and $\delta_k = 0$ for $k \neq 0$.

COROLLARY 3.6 (positive definiteness of the weight matrix $\Gamma$). *Assume that the structure of $\mathcal{S}$ is given by* (2.6) *with the block $C^{(q)}$ being block-Toeplitz, block-Hankel, or unstructured and having at least $d$ columns. Then the matrix $\Gamma(X)$ is positive definite for all $X \in \mathbb{R}^{n \times d}$.*

*Proof.* We will show that $\Gamma^{(q)}(X) > 0$ for all $X \in \mathbb{R}^{n\times d}$. From (3.2), it follows that $\Gamma$ has the same property. By the assumption $\operatorname{col dim}(C^{(q)}) \geq d$, it follows that $X_{\text{ext}}^{(q)} = \left[\begin{smallmatrix} * \\ -I_d \end{smallmatrix}\right]$, where the $*$ denotes a block (possibly empty) depending on $X$. In the unstructured case, $\Gamma^{(q)} = I_m \otimes (X_{\text{ext}}^{(q)\top} X_{\text{ext}}^{(q)})$; see (3.6). But $\operatorname{rank}(X_{\text{ext}}^{(q)\top} X_{\text{ext}}^{(q)}) = d$, so that $\Gamma^{(q)}$ is nonsingular. In the block-Hankel/Toeplitz case, $G^{(q)}$ is block-Toeplitz and block-banded; see Lemmas 3.4 and 3.5. One can verify by inspection that independent of $X$, $G^{(q)}(X)$ has full row rank due to its row echelon form. Then $\Gamma^{(q)} = G^{(q)} G^{(q)\top} > 0$. ∎

The positive definiteness of $\Gamma$ is studied in a statistical setting in [10, sect. 4], where more general conditions are given. The restriction of (2.6) that ensures $\Gamma > 0$ is fairly minor, so that in what follows we will consider STLS problems of this type and replace the pseudoinverse in (2.5) with the inverse.

In the next section, we give an interpretation of Theorem 3.1 from a statistical point of view, and in section 5 we consider in more detail the algorithmic side of the problem.

**4. Stochastic interpretation.** Our work on the STLS problem has its origin in the field of estimation theory. A linear multivariate *errors-in-variables* (EIV) model is defined as follows:

$$AX \approx B, \quad \text{where} \quad A = \bar{A} + \tilde{A}, \quad B = \bar{B} + \tilde{B}, \quad \text{and} \quad \bar{A}\bar{X} = \bar{B}. \tag{4.1}$$

The observations $A$ and $B$ are obtained from (nonstochastic) *true values* $\bar{A}$ and $\bar{B}$ with *measurement errors* $\tilde{A}$ and $\tilde{B}$ that are zero mean random matrices. Define the extended matrix $\tilde{C} := \begin{bmatrix}\tilde{A} & \tilde{B}\end{bmatrix}$ and the vector $\tilde{c} := \text{vec}(\tilde{C}^\top)$ of the measurement errors. It is well known (see [25, Chap. 8]) that the TLS problem (1.1) provides a consistent estimator for the true value of the parameter $\bar{X}$ in the EIV model (4.1) if $\text{cov}(\tilde{c}) = \sigma^2 I$ (and additional technical conditions are satisfied). If, in addition to $\text{cov}(\tilde{c}) = \sigma^2 I$, $\tilde{c}$ is normally distributed, i.e., $\tilde{c} \sim \text{N}(0, \sigma^2 I)$, then the solution $\hat{X}_{\text{tls}}$ of the TLS problem is the maximum likelihood estimate of $\bar{X}$.

The EIV model (4.1) is called the *structured errors-in-variables model* if the observed data $C$ and the true value $\bar{C} := \begin{bmatrix}\bar{A} & \bar{B}\end{bmatrix}$ have a structure defined by a function $\mathcal{S}$. Therefore,

$$C = \mathcal{S}(p) \quad \text{and} \quad \bar{C} = \mathcal{S}(\bar{p}),$$

where $\bar{p} \in \mathbb{R}^{n_p}$ is a (nonstochastic) true value of the parameter $p$. As a consequence the matrix of measurement errors is also structured. Let $\mathcal{S}$ be affine (2.2). Then

$$\tilde{C} = \sum_{i=1}^{n_p} S_i \tilde{p}_i \qquad \text{and} \qquad p = \bar{p} + \tilde{p},$$

where the random vector $\tilde{p}$ represents the measurement error on the structure parameter $\bar{p}$. In [10], it is proven that the STLS problem (2.1) provides a consistent estimator for the true value of the parameter $\bar{X}$ if $\text{cov}(\tilde{p}) = \sigma^2 I$ (and additional technical conditions are satisfied). If $\tilde{p} \sim \text{N}(0, \sigma^2 I)$, then a solution $\hat{X}$ of the STLS problem is a maximum likelihood estimate of $\bar{X}$.

Let $\tilde{r}(X) := \text{vec}\big(\mathcal{S}(\tilde{p}) X_{\text{ext}}\big)$ be the random part of the residual $r$. In the stochastic setting, the weight matrix $\Gamma$ is up to the scale factor $\sigma^2$ equal to the covariance matrix $V_{\tilde{r}} := \text{cov}(\tilde{r})$. Indeed, $\tilde{r} = G\tilde{p}$, so that

$$V_{\tilde{r}} := \mathbf{E}\, \tilde{r}\tilde{r}^\top = G\, \mathbf{E}\, (\tilde{p}\tilde{p}^\top) G^\top = \sigma^2 G G^\top = \sigma^2 \Gamma.$$

Next we show that the structure of $\Gamma$ is in a one-to-one correspondence with the structure of $V_{\tilde{c}} := \text{cov}(\tilde{c})$. Let $\Gamma_{ij} \in \mathbb{R}^{dK \times dK}$ be the $(i,j)$th block of $\Gamma$ and let $V_{\tilde{\mathbf{c}},ij} \in \mathbb{R}^{(n+d)K \times (n+d)K}$ be the $(i,j)$th block of $V_{\tilde{c}}$. Define also the following partitionings of the vectors $\tilde{r}$ and $\tilde{c}$:

$$\tilde{r} =: \begin{bmatrix} \tilde{\mathbf{r}}_1 \\ \vdots \\ \tilde{\mathbf{r}}_{\mathbf{m}} \end{bmatrix}, \quad \tilde{\mathbf{r}}_i \in \mathbb{R}^{dK} \qquad \text{and} \qquad \tilde{c} =: \begin{bmatrix} \tilde{\mathbf{c}}_1 \\ \vdots \\ \tilde{\mathbf{c}}_{\mathbf{m}} \end{bmatrix}, \quad \tilde{\mathbf{c}}_i \in \mathbb{R}^{(n+d)K},$$

where $\mathbf{m} := m/K$. Using $\mathbf{r}_i = \mathbf{X}_{\text{ext}} \mathbf{c}_i$, where $\mathbf{X}_{\text{ext}} := (I_K \otimes X_{\text{ext}}^\top)$, we have

$$\sigma^2 \Gamma_{ij} = \mathbf{E}\, \tilde{\mathbf{r}}_i \tilde{\mathbf{r}}_j^\top = \mathbf{X}_{\text{ext}} \mathbf{E}\, (\tilde{\mathbf{c}}_i \tilde{\mathbf{c}}_j^\top) \mathbf{X}_{\text{ext}}^\top = \mathbf{X}_{\text{ext}} V_{\tilde{\mathbf{c}},ij} \mathbf{X}_{\text{ext}}^\top. \tag{4.2}$$

The one-to-one relation between the structures of $\Gamma$ and $V_{\tilde{c}}$ allows us to relate the structural properties of $\Gamma$, established in Theorem 3.1, with statistical properties of the measurement errors. Define stationarity and $s$-dependence of a centered sequence of random vectors $\tilde{\mathbf{c}} := \{\tilde{\mathbf{c}}_1, \tilde{\mathbf{c}}_2, \dots\}$, $\tilde{\mathbf{c}}_i \in \mathbb{R}^{(n+d)K}$ as follows:

- $\tilde{\mathbf{c}}$ is *stationary* if the covariance matrix $V_{\tilde{c}}$ is block-Toeplitz with block size $(n+d)K \times (n+d)K$.

- $\tilde{\mathbf{c}}$ is *s-dependent* if the covariance matrix $V_{\tilde{c}}$ is block-banded with block size $(n+d)K \times (n+d)K$ and block bandwidth $2s+1$.

The sequence of measurement errors $\tilde{\mathbf{c}}$ being stationary and $s$-dependent corresponds to $\Gamma$ being block-Toeplitz and block-banded.

The statistical setting gives an insight into the relation between the structure of the weight matrix $\Gamma$ and the structure of the data matrix $C$. It can be verified that the structure specification (2.6) implies stationarity and $s$-dependence for $\tilde{\mathbf{c}}$. This indicates an alternative (statistical) proof of Theorem 3.1; see the technical report [14].

The blocks of $\Gamma$ are quadratic functions of $X$, $\Gamma_{ij}(X) = \mathbf{X}_{\text{ext}} W_{\tilde{\mathbf{c}},ij} \mathbf{X}_{\text{ext}}^\top$, where $W_{\tilde{\mathbf{c}},ij} := V_{\tilde{\mathbf{c}},ij}/\sigma^2$; see (4.2). Moreover, by Theorem 3.1, we have that under assumption (2.6), $W_{\tilde{\mathbf{c}},ij} = W_{\tilde{\mathbf{c}},|i-j|}$ for certain matrices $W_{\tilde{\mathbf{c}},k}$, $k = 1, \dots, \mathbf{m}$, and $W_{\tilde{\mathbf{c}},ij} = 0$ for $|i-j| > s$, where $s$ is defined in Theorem 3.1. Therefore,

$$\Gamma_k(X) = \mathbf{X}_{\text{ext}} W_{\tilde{\mathbf{c}},k} \mathbf{X}_{\text{ext}}^\top \quad \text{for } k = 0, 1, \dots, s, \quad \text{where} \quad W_{\tilde{\mathbf{c}},k} := \frac{1}{\sigma^2} V_{\tilde{\mathbf{c}},k}.$$

In (3.6) we show how the matrices $\{\Gamma_k\}_{k=0}^s$ can be determined from the structure specification (2.6). Similar expressions can be written for the matrices $\{W_{\tilde{\mathbf{c}},k}\}_{k=0}^s$.

In the computational algorithm described in section 5, we use the partitioning of the matrix $\Gamma$ into blocks of size $d \times d$. Let $\Gamma_{ij} \in \mathbb{R}^{d\times d}$ be the $(i,j)$th block of $\Gamma$ and let $V_{\tilde{c},ij} \in \mathbb{R}^{(n+d)\times(n+d)}$ be the $(i,j)$th block of $V_{\tilde{c}}$. Define the following partitionings of the vectors $\tilde{r}$ and $\tilde{c}$:

$$\tilde{r} =: \begin{bmatrix} \tilde{r}_1 \\ \vdots \\ \tilde{r}_m \end{bmatrix}, \quad r_i \in \mathbb{R}^d \qquad \text{and} \qquad \tilde{c} =: \begin{bmatrix} \tilde{c}_1 \\ \vdots \\ \tilde{c}_m \end{bmatrix}, \quad c_i \in \mathbb{R}^{n+d}.$$

Using $r_i = X_{\text{ext}}^\top c_i$, we have

$$\Gamma_{ij} = \frac{1}{\sigma^2} \mathbf{E}\, \tilde{r}_i \tilde{r}_j^\top = \frac{1}{\sigma^2} X_{\text{ext}}^\top \mathbf{E}\,(\tilde{c}_i \tilde{c}_j^\top) X_{\text{ext}} = \frac{1}{\sigma^2} X_{\text{ext}}^\top V_{\tilde{c},ij} X_{\text{ext}} =: X_{\text{ext}}^\top W_{\tilde{c},ij} X_{\text{ext}}.$$

**5. Efficient cost function and first derivative evaluation.** We consider an efficient numerical method for solving the STLS problem (2.1) by applying standard local optimization algorithms to the equivalent problem (2.5). With this approach, the main computational effort is in the cost function and its first derivative evaluation.

First, we describe the evaluation of the cost function: given $X$, compute $f_0(X)$. For given $X$, and with $\{\Gamma_k\}_{k=0}^s$ constructed as described in the proof of Theorem 3.1, the weight matrix $\Gamma(X)$ is specified. Then from the solution of the system $\Gamma(X) y_r(X) = r(X)$, the cost function is found as $f_0(X) = r^\top(X) y_r(X)$.

The properties of $\Gamma(X)$ can be exploited in the solution of the system $\Gamma y_r = r$. The subroutine `MB02GD` from the SLICOT library [2] exploits both the block-Toeplitz and the banded structure to compute a Cholesky factor of $\Gamma$ in $O((dK)^2 sm)$ flops. In combination with the LAPACK subroutine `DPBTRS` that solves block-banded triangular systems of equations, the cost function is evaluated in $O(m)$ flops. Thus an algorithm for local optimization that uses only cost function evaluations has computational complexity $O(m)$ flops per iteration, because the computations needed internally for the optimization algorithm do not depend on $m$.

Next, we describe the evaluation of the derivative. The derivative of the cost function $f_0$ is (see the appendix)

$$f_0'(X) = 2 \sum_{i,j=1}^{m} a_j r_i^\top(X) M_{ij}(X) - 2 \sum_{i,j=1}^{m} \begin{bmatrix} I & 0 \end{bmatrix} W_{\tilde{c},ij} \begin{bmatrix} X \\ -I \end{bmatrix} N_{ji}(X), \tag{5.1}$$

where $A^\top =: \begin{bmatrix} a_1 & \cdots & a_m \end{bmatrix}$, with $a_i \in \mathbb{R}^n$,

$$M(X) := \Gamma^{-1}(X), \qquad N(X) := \Gamma^{-1}(X) r(X) r^\top(X) \Gamma^{-1}(X),$$

and $M_{ij} \in \mathbb{R}^{d\times d}$, $N_{ij} \in \mathbb{R}^{d\times d}$ are the $(i,j)$th blocks of $M$ and $N$, respectively.

Consider the two partitionings of $y_r \in \mathbb{R}^{md}$,

$$y_r =: \begin{bmatrix} y_{r,1} \\ \vdots \\ y_{r,m} \end{bmatrix}, \quad y_{r,i} \in \mathbb{R}^d \qquad \text{and} \qquad y_r =: \begin{bmatrix} \mathbf{y}_{r,1} \\ \vdots \\ \mathbf{y}_{r,\mathbf{m}} \end{bmatrix}, \quad \mathbf{y}_{r,i} \in \mathbb{R}^{dK}, \tag{5.2}$$

where $\mathbf{m} := m/K$. The first sum in (5.1) becomes

$$\sum_{i,j=1}^{m} a_j r_i^\top M_{ij} = A^\top Y_r, \quad \text{where} \quad Y_r^\top := \begin{bmatrix} y_{r,1} & \cdots & y_{r,m} \end{bmatrix}. \tag{5.3}$$

Define the sequence of matrices

$$\mathbf{N}_k := \sum_{i=1}^{\mathbf{m}-k} \mathbf{y}_{r,i+k} \mathbf{y}_{r,i}^\top, \quad \mathbf{N}_k = \mathbf{N}_{-k}^\top, \quad k = 0, \dots, s.$$

The second sum in (5.1) can be written as

$$\sum_{i,j=1}^{m} \begin{bmatrix} I & 0 \end{bmatrix} W_{\tilde{c},ij} \begin{bmatrix} X \\ -I \end{bmatrix} N_{ji} = \sum_{k=-s}^{s} \sum_{i,j=1}^{K} (W_{\tilde{\mathbf{a}},k,ij} X - W_{\tilde{\mathbf{a}}\tilde{\mathbf{b}},k,ij}) \mathbf{N}_{k,ij}^\top,$$

where $W_{\tilde{\mathbf{c}},k,ij} \in \mathbb{R}^{(n+d)\times(n+d)}$ is the $(i,j)$th block of $W_{\tilde{\mathbf{c}},k} \in \mathbb{R}^{K(n+d)\times K(n+d)}$, $W_{\tilde{\mathbf{a}},k,ij} \in \mathbb{R}^{n\times n}$ and $W_{\tilde{\mathbf{a}}\tilde{\mathbf{b}},k,ij} \in \mathbb{R}^{n\times d}$ are defined as blocks of $W_{\tilde{\mathbf{c}},k,ij}$ as

$$W_{\tilde{\mathbf{c}},k,ij} =: \begin{bmatrix} W_{\tilde{\mathbf{a}},k,ij} & W_{\tilde{\mathbf{a}}\tilde{\mathbf{b}},k,ij} \\ W_{\tilde{\mathbf{b}}\tilde{\mathbf{a}},k,ij} & W_{\tilde{\mathbf{b}},k,ij} \end{bmatrix},$$

and $\mathbf{N}_{k,ij} \in \mathbb{R}^{d\times d}$ is the $(i,j)$th block of $\mathbf{N}_k \in \mathbb{R}^{dK\times dK}$.

Thus the evaluation of the derivative $f_0'(X)$ uses the solution of $\Gamma y_r = r$, already computed for the cost function evaluation and additional operations of $O(m)$ flops. The steps described above are summarized in Algorithm 1.

**Algorithm 1.** Cost function and first derivative evaluation.

1: Input: $A$, $B$, $X$, $\{W_{\tilde{\mathbf{c}},k}\}_{k=0}^s$.
2: $\Gamma_k = (I_K \otimes X_{\text{ext}}^\top) W_{\tilde{\mathbf{c}},k} (I_K \otimes X_{\text{ext}}^\top)^\top$ for $k = 0, 1, \dots, s$,
3: $r = \text{vec}\big((AX - B)^\top\big)$,
4: solve (via `MB02GD` and `DPBTRS`) $\Gamma y_r = r$, where $\Gamma$ is given in (3.1),
5: $f_0 = r^\top y_r$.
6: If only the cost function evaluation is required, output $f_0$ and stop.
7: $\mathbf{N}_k = \sum_{i=1}^{\mathbf{m}-k} \mathbf{y}_{r,i+k} \mathbf{y}_{r,i}^\top$ for $k = 0, 1, \dots, s$, where $\mathbf{y}_i$ is defined in (5.2).
8: $f_0' = 2A^\top Y_r - 2\sum_{k=-s}^{s} \sum_{i,j=1}^{K} (W_{\tilde{\mathbf{a}},k,ij} X - W_{\tilde{\mathbf{a}}\tilde{\mathbf{b}},k,ij}) \mathbf{N}_{k,ij}^\top$, where $Y_r$ is defined in (5.3).
9: Output $f_0$, $f_0'$ and stop.

The flops per step for Algorithm 1 are as follows:

2. $(n+d)(n+2d)dK^3$.
3. $m(n+1)d$.
4. $msd^2K^2$.
5. $md$.
7. $msd^2K - s(s+1)d^2K^2/2$.
8. $mnd + (2s+1)(nd+n+1)dK^2$.

Thus in total $O(md(sdK^2+n) + n^2dK^3 + 3nd^2K^3 + 2d^3K^3 + 2snd^2K^2)$ flops are required for cost function and first derivative evaluation. Note that the flop counts depend on the structure through $s$.

Using the computation of the cost function and its first derivative, as outlined above, we can apply the BFGS (Broyden, Fletcher, Goldfarb, and Shanno) quasi-Newton method. A more efficient alternative, however, is to apply a nonlinear least squares optimization algorithm, such as the Levenberg–Marquardt algorithm. Let $\Gamma = U^\top U$ be the Cholesky factorization of $\Gamma$. Then $f = F^\top F$, with $F := U^{-1}r$. (Note that the evaluation of $F(X)$ is cheaper than that of $f(X)$.) We do not know an analytic expression for the Jacobian matrix $J(X) = [\partial F_i/\partial x_j]$, but instead we use the so-called pseudo-Jacobian $J_+$ proposed in [9]. The evaluation of $J_+$ can be done efficiently, using the approach described above for $f'(X)$.

Moreover, by using the nonlinear least squares approach and the pseudo-Jacobian $J_+$, we have as a byproduct of the optimization algorithm an estimate of the covariance matrix $V_{\hat{x}} = \mathbf{E}\left(\operatorname{vec}(\hat{X})\operatorname{vec}^\top(\hat{X})\right)$. As shown in [19, Chap. 17.4.7, eqns. (17)–(35)], $V_{\hat{x}} \approx \left(J_+^\top(\hat{X})J_+(\hat{X})\right)^{-1}$. Using $V_{\hat{x}}$, we can compute statistical confidence bounds for the estimate $\hat{X}$.

**6. Applications and simulation examples.** Under assumption (2.6), the specification of $\mathcal{S}$ is given by $K$ and the array $\mathcal{D} \in \{(\mathtt{T},\mathtt{H},\mathtt{U},\mathtt{E}) \times \mathbb{N} \times \mathbb{N}\}^q$ that describes the structure of the blocks $\{C^{(l)}\}_{l=1}^q$; $\mathcal{D}_l$ specifies the block $C^{(l)}$ by giving its type $\mathcal{D}_l(1)$ ($\mathtt{T}$ = block-Toeplitz, $\mathtt{H}$ = block-Hankel, $\mathtt{U}$ = unstructured, and $\mathtt{E}$ = exact), the number of columns $n_l = \mathcal{D}_l(2)$, and, for block-Toeplitz/Hankel blocks, the column dimension $\mathcal{D}_l(3)$ of the block. The following well-known problems are special cases of the block-Toeplitz/Hankel STLS problem of this paper for particular choices of the structure description $\mathcal{D}$. (If not specified, $K$ and the third element of $\mathcal{D}_l$ are equal to one.)

1. *Least squares problem:* $AX \approx B$, $A \in \mathbb{R}^{m\times n}$ exact, $B \in \mathbb{R}^{m\times d}$ noisy and unstructured is achieved by $\mathcal{D} = [[\mathtt{E}\ n], [\mathtt{U}\ d]]$.

2. *TLS problem:* $AX \approx B$, $C = [A\ B] \in \mathbb{R}^{m\times(n+d)}$ noisy and unstructured is achieved by $\mathcal{D} = [\mathtt{U}\ n+d]$.

3. *Data least squares problem* [3]: $AX \approx B$, $A \in \mathbb{R}^{m\times n}$ noisy and unstructured, and $B \in \mathbb{R}^{m\times d}$ exact is achieved by $\mathcal{D} = [[\mathtt{U}\ n], [\mathtt{E}\ d]]$.

4. *Mixed LS-TLS problem* [25, sect. 3.5]: $AX \approx B$, $A = [A_{\text{noisy}}\ A_{\text{exact}}]$, $A_{\text{noisy}} \in \mathbb{R}^{m\times n_1}$ and $B \in \mathbb{R}^{m\times d}$ noisy and unstructured, $A_{\text{exact}} \in \mathbb{R}^{m\times n_2}$ exact is achieved by $\mathcal{D} = [[\mathtt{U}\ n_1], [\mathtt{E}\ n_2], [\mathtt{U}\ d]]$.

5. *Hankel low-rank approximation problem* [4, sect. 4.5], [21]:

$$\min_{\Delta p} \|\Delta p\|^2 \quad \text{subject to} \quad \mathcal{H}(p - \Delta p) \text{ has given rank } n, \tag{6.1}$$

where $\mathcal{H}$ is a mapping from the parameter space $\mathbb{R}^{n_p}$ to the set of the $m \times (n+d)$ block-Hankel matrices, with block size $n_y \times n_u$. If the rank constraint is expressed as

$\mathcal{H}(\hat{p}) \left[\begin{smallmatrix} X \\ -I \end{smallmatrix}\right] = 0$, with $X \in \mathbb{R}^{n \times d}$ an additional variable, then (6.1) becomes an STLS problem with $K = n_y$ and $\mathcal{D} = \{[\mathtt{H}\ n + d\ n_u]\}$.

6. *Deconvolution problem:* For a description of the problem and its formulation as an STLS problem, see [17]. In [17] a finite impulse response (FIR) filter identification problem is considered, which is an application of deconvolution for system identification. The structure in this case is $\mathcal{D} = [[\mathtt{T}\ n], [\mathtt{U}\ 1]]$, where $n$ is the number of lags of the FIR filter.

7. *Transfer function estimation:* For a description of the problem and its formulation as an STLS problem, see [4, sect. 4.6]. The structure arising in this problem is $\mathcal{D} = [[\mathtt{H}\ n_b + 1], [\mathtt{H}\ n_a + 1]]$, where $n_b$ is the order of the numerator and $n_a$ is the order of the denominator of the estimated transfer function.

The last three problems have system theoretic interpretation—the Hankel–low-rank approximation problem is a *noisy realization problem* [5] or alternatively a model reduction problem (see section 6.2), and the deconvolution and the transfer function estimation problems are system identification problems (see section 6.1). For multi-input, multi-output (MIMO) systems, these problems result in block-Toeplitz/Hankel structured matrices.

Next we show simulation examples for the system identification and model reduction applications. They aim to illustrate the applicability of the derived algorithm for real-life problems. More details on the application of STLS for these problems and more realistic identification examples can be found in [16].

**6.1. Improvement of the subspace identification estimate.** Maximum likelihood SISO transfer function identification from noisy input/output data can be formulated as an STLS problem with a data matrix composed of two Hankel or Toeplitz structured blocks next to each other; see [4, sect. 4.6]. The STLS method, however, needs a good initial approximation. On the other hand, the popular subspace identification methods [26] do not need initial approximation but do not minimize a particular cost function. As a result, in general, they are statistically not as accurate as the methods based on the maximum likelihood principle. A natural idea is to use the subspace method estimate, on a second stage of the estimation problem, as an initial approximation for the STLS method. The latter is expected to reduce the estimation error.

We show a simulation example to illustrate the idea. Consider the linear time-invariant (LTI) system with a transfer function

$$\bar{H}(z) = 0.151 \cdot \frac{1 + 0.9z + 0.49z^2 + 0.145z^3}{1 - 1.2z + 0.81z^2 - 0.27z^3}.$$

This is the "true model" that we aim to identify. Let $(\bar{u}(t), \bar{y}(t))_{t=1}^m$ be an input/output trajectory of the system, where $\bar{u}$ is a zero mean, white process with unit variance. The data available for the identification are $(u(t), y(t))_{t=1}^m$, where $u = \bar{u} + \tilde{u}$, $y = \bar{y} + \tilde{y}$, and $\tilde{u}$, $\tilde{y}$ are zero mean, normal, white, measurement noise, with variance $\sigma^2 = 0.05^2$. Assuming that the exact system order is known, we apply the state space algorithm N4SID [26]. The obtained estimate is used as an initial approximation for the STLS algorithm.

Let vec_par be an operator that stacks the parameters of a transfer function, i.e., the coefficients of the numerator and denominator, in a vector. We define the average relative error of estimation by

$$\bar{e}_{\text{par}} = \frac{1}{N} \sum_{k=1}^{N} \frac{\|\text{vec\_par}(\bar{H}) - \text{vec\_par}(\hat{H}^{(k)})\|_2}{\|\text{vec\_par}(\bar{H})\|_2}.$$

Here $\hat{H}^{(k)}$ denotes the identified transfer function in the $k$th repetition of the experiment; $N = 100$ repetitions of the experiment with different measurement noise realizations are performed. Figure 6.1 shows the average relative errors $\bar{e}_{\text{par}}$ for the subspace method and for the STLS-based maximum likelihood method as a function of the time horizon $m$. The example shows that, for large sample sizes, the two approaches give close estimates and, for small sample sizes, the subspace estimate can be improved by the STLS method.

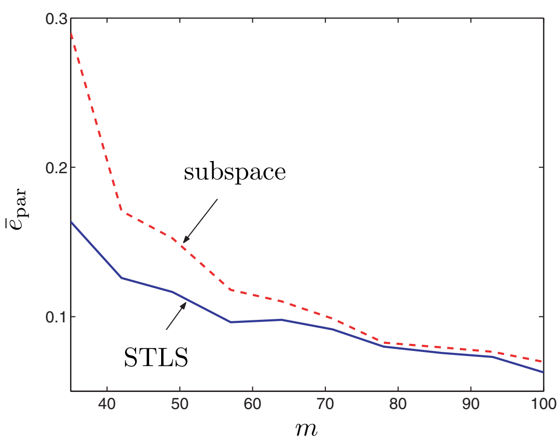


FIG. 6.1. *Results for the system identification example: Average relative error of estimation for the subspace and STLS methods.*

**6.2. MIMO system model reduction.** Finite horizon 2-norm optimal model reduction can be formulated as an STLS problem with a block-Hankel structured data matrix. On the other hand, balanced model reduction [18], like subspace identification, does not require initial approximation but also does not minimize a particular cost function. Again an improvement can be expected over the balanced model reduction method when the STLS method is used on a second stage of the approximation.

To illustrate the idea, consider the following example. A 10th order, 2-input, 1-output random system has to be approximated by an $r$th order system, where $r = 2, 4, 6, 8$. First we apply balanced reduction. The obtained solution is used as an initial approximation for the STLS method. Table 6.1 shows the average relative $\mathcal{H}_2$-errors of approximation over $N = 100$ repetitions:

$$\bar{e}_{\mathcal{H}_2} = \frac{1}{N} \sum_{k=1}^{N} \frac{\|\bar{H} - \hat{H}^{(k)}\|_{\mathcal{H}_2}}{\|\bar{H}\|_{\mathcal{H}_2}}.$$

The example confirms that the STLS method can be used to improve the result of the balanced model reduction method.

TABLE 6.1
*Results for the model reduction example: Average relative error of estimation $\bar{e}_{\mathcal{H}_2}$ for balanced model reduction (BMR) and STLS.*

| Method | $r = 2$ | $r = 4$ | $r = 6$ | $r = 8$ |
|---|---|---|---|---|
| BMR | 0.1062122 | 0.0288455 | 0.0012585 | 0.0000259 |
| STLS | 0.1034344 | 0.0276010 | 0.0012433 | 0.0000229 |

**7. Conclusions.** We considered an STLS problem with the structure of the data matrix, specified blockwise. Each of the blocks can be block-Toeplitz/Hankel structured, unstructured, or exact. It was shown that such a formulation is flexible and covers as special cases many previously studied structured and unstructured matrix approximation problems.

The numerical solution method of [13] was extended to the block-Toeplitz/Hankel case. The approach is based on an equivalent unconstrained optimization problem: $\min_X r^\top(X)\Gamma^{-1}(X)r(X)$. We proved that under assumption (2.6) about the structure of the data matrix, the weight matrix $\Gamma$ is block-Toeplitz and block-banded. These properties were used for cost function and first derivative evaluation with computational cost linear in the sample size.

The extension to block-Toeplitz/Hankel structured matrices is motivated by identification and model reduction problems for MIMO dynamical systems. Useful further extensions are (i) to consider a weighted quadratic cost function $\Delta p^\top V \Delta p$, with $V > 0$ diagonal, and (ii) regularized STLS problems, where the cost function is augmented with the regularization term $\mathrm{vec}^\top(X)Q\mathrm{vec}(X)$. These extensions are still computable in $O(m)$ flops per iteration.

**Appendix. Derivation of the first derivative of the cost function $\boldsymbol{f_0}$.** Denote by $D$ the differential operator. It acts on a differentiable function $f_0 : U \to \mathbb{R}$, where $U$ is an open set in $\mathbb{R}^{n\times d}$ and gives as a result another function, the differential of $f_0$, $D(f_0) : U \times \mathbb{R}^{n\times d} \to \mathbb{R}$. The differential $D(f_0)$ is linear in its second argument, i.e.,

$$D(f_0) := \mathrm{d}f_0(X, H) = \mathrm{trace}\big(f_0'(X)H^\top\big), \tag{A.1}$$

and has the property

$$f_0(X + H) = f_0(X) + \mathrm{d}f_0(X, H) + \mathrm{o}(\|H\|_\mathrm{F})$$

for all $X \in U$ and for all $H \in \mathbb{R}^{n\times d}$. (The notation $\mathrm{o}(\|H\|_\mathrm{F})$ has the usual meaning: $g(H) = \mathrm{o}(\|H\|_\mathrm{F})$ if and only if $\lim_{\|H\|_\mathrm{F}\to 0} g(H)/\|H\|_\mathrm{F} = 0$.) The function $f_0' : U \to \mathbb{R}^{n\times l}$ is the derivative of $f_0$. We compute it by deriving the differential $D(f_0)$ and representing it in the form (A.1), from which $f_0'(X)$ is extracted.

The differential of the cost function $f_0(X) = r^\top(X)\Gamma^{-1}(X)r(X)$ is (using the rule for differentiation of an inverse matrix)

$$\mathrm{d}f_0(X, H) = 2r^\top\Gamma^{-1}\begin{bmatrix} H^\top a_1 \\ \vdots \\ H^\top a_m \end{bmatrix} - r^\top\Gamma^{-1}\big(\mathrm{d}\Gamma(X, H)\big)\Gamma^{-1}r.$$

The differential of the weight matrix

$$\Gamma = V_{\tilde r} = \mathbf{E}\,\tilde r\tilde r^\top = \mathbf{E}\begin{bmatrix} X^\top\tilde a_1 - \tilde b_1 \\ \vdots \\ X^\top\tilde a_m - \tilde b_m \end{bmatrix}\begin{bmatrix} \tilde a_1^\top X - \tilde b_1^\top & \cdots & \tilde a_m^\top X - \tilde b_m^\top \end{bmatrix},$$

where $\tilde A^\top =: \begin{bmatrix} \tilde a_1 & \cdots & a_m \end{bmatrix}$, $\tilde a_i \in \mathbb{R}^n$, and $\tilde B^\top =: \begin{bmatrix} \tilde b_1 & \cdots & b_m \end{bmatrix}$, $\tilde b_i \in \mathbb{R}^d$, is

$$\mathrm{d}\Gamma(X, H) = \mathbf{E}\begin{bmatrix} H^\top\tilde a_1 \\ \vdots \\ H^\top\tilde a_m \end{bmatrix}\tilde r^\top + \mathbf{E}\,\tilde r\begin{bmatrix} \tilde a_1^\top H & \cdots & \tilde a_m^\top H \end{bmatrix}. \tag{A.2}$$

With $M_{ij} \in \mathbb{R}^{d\times d}$ denoting the $(i,j)$th block of $\Gamma^{-1}$,

$$\begin{aligned}\frac{1}{2}\mathrm{d}f_0(X,H) &= \sum_{i,j=1}^{m} r_i^\top M_{ij} H^\top a_j - \sum_{i,j,k,l=1}^{m} r_l^\top M_{li} H^\top \mathbf{E}\, \tilde{a}_i \tilde{c}_j^\top X_{\mathrm{ext}} M_{jl} r_l \\ &= \operatorname{trace}\Bigg(\Bigg( \sum_{i,j=1}^{m} a_j r_i^\top M_{ij} - \sum_{i,j,k,l=1}^{m} \begin{bmatrix} I & 0 \end{bmatrix} V_{\tilde{c},ij} X_{\mathrm{ext}} M_{jl} r_l r_l^\top M_{li} \Bigg) H^\top \Bigg),\end{aligned}$$

so that

$$\frac{1}{2} f_0'(X) = \sum_{i,j=1}^{m} a_j r_i^\top M_{ij} - \sum_{i,j=1}^{m} \begin{bmatrix} I & 0 \end{bmatrix} V_{\tilde{c},ij} X_{\mathrm{ext}} N_{ji},$$

where $N_{ji}(X) := \sum_{l=1}^{m} M_{jl} r_l \cdot \sum_{l=1}^{m} r_l^\top M_{li}$.

**Acknowledgments.** We would like to thank A. Kukush, M. Schuermans, P. Lemmerling, N. Mastronardi, and D. Sima for helpful discussion on the STLS problem.

## REFERENCES


[1] T. Abatzoglou, J. Mendel, and G. Harada, *The constrained total least squares technique and its application to harmonic superresolution*, IEEE Trans. Signal Process., 39 (1991), pp. 1070–1087.

[2] P. Benner, V. Mehrmann, V. Sima, S. Van Huffel, and A. Varga, *SLICOT—a subroutine library in systems and control theory*, in Applied and Computational Control, Signal and Circuits, Vol. 1, B. N. Datta, ed., Birkhäuser, Boston, 1999, Chap. 10, pp. 499–539.

[3] G. Cirrincione, G. Ganesan, K. Hari, and S. Van Huffel, *Direct and neural techniques for the data least squares problem*, in Proceedings of the International Symposium on the Mathematical Theory of Networks and Systems (MTNS), Perpignan, France, 2000.

[4] B. De Moor, *Structured total least squares and $L_2$ approximation problems*, Linear Algebra Appl., 188–189 (1993), pp. 163–207.

[5] B. De Moor, *Total least squares for affinely structured matrices and the noisy realization problem*, IEEE Trans. Signal Process., 42 (1994), pp. 3104–3113.

[6] B. De Moor and B. Roorda, *$L_2$-optimal linear system identification structured total least squares for SISO systems*, in Proceedings of the 33th Conference on Decision and Control (CDC), Lake Buena Vista, FL, IEEE Control Systems Society, 1994, pp. 2874–2879.

[7] W. A. Fuller, *Measurement Error Models*, John Wiley, New York, 1987.

[8] G. H. Golub and C. F. Van Loan, *An analysis of the total least squares problem*, SIAM J. Numer. Anal., 17 (1980), pp. 883–893.

[9] P. Guillaume and R. Pintelon, *A Gauss–Newton-like optimization algorithm for "weighted" nonlinear least-squares problems*, IEEE Trans. Signal Process., 44 (1996), pp. 2222–2228.

[10] A. Kukush, I. Markovsky, and S. Van Huffel, *Consistency of the structured total least squares estimator in a multivariate errors-in-variables model*, J. Statist. Plann. Inference, to appear.

[11] P. Lemmerling, N. Mastronardi, and S. V. Huffel, *Fast algorithm for solving the Hankel/Toeplitz structured total least squares problem*, Numer. Algorithms, 23 (2000), pp. 371–392.

[12] M. J. Levin, *Estimation of a system pulse transfer function in the presence of noise*, IEEE Trans. Automat. Control, 9 (1964), pp. 229–235.

[13] I. Markovsky, S. Van Huffel, and A. Kukush, *On the computation of the multivariate structured total least squares estimator*, Numer. Linear Algebra Appl., 11 (2004), pp. 591–608.

[14] I. Markovsky, S. Van Huffel, and R. Pintelon, *Block-Toeplitz/Hankel Structured Total Least Squares*, Tech. Rep. 03–135, Department of Electrical Engineering, K.U. Leuven, Belgium, 2003.

[15] I. Markovsky, S. Van Huffel, and R. Pintelon, *Software for Structured Total Least Squares Estimation: User's Guide*, Tech. Rep. 03–136, Department of Electrical Engineering, K.U. Leuven, Belgium, 2003.

[16] I. Markovsky, J. C. Willems, S. Van Huffel, B. D. Moor, and R. Pintelon, *Application of Structured Total Least Squares for System Identification and Model Reduction*, Tech. Rep. 04–51, Department of Electrical Engineering, K.U. Leuven, Belgium, 2004.

[17] N. Mastronardi, P. Lemmerling, and S. Van Huffel, *Fast structured total least squares algorithm for solving the basic deconvolution problem*, SIAM J. Matrix Anal. Appl., 22 (2000), pp. 533–553.

[18] B. C. Moore, *Principal component analysis in linear systems: Controllability, observability and model reduction*, IEEE Trans. Automat. Control, 26 (1981), pp. 17–31.

[19] R. Pintelon and J. Schoukens, *System Identification: A Frequency Domain Approach*, IEEE Press, Piscataway, NJ, 2001.

[20] J. B. Rosen, H. Park, and J. Glick, *Total least norm formulation and solution for structured problems*, SIAM J. Matrix Anal. Appl., 17 (1996), pp. 110–126.

[21] M. Schuermans, P. Lemmerling, and S. Van Huffel, *Structured weighted low rank approximation*, Numer. Linear Algebra Appl., 11 (2004), pp. 609–618.

[22] S. Van Huffel, ed., *Recent Advances in Total Least Squares Techniques and Errors-in-Variables Modeling*, SIAM, Philadelphia, 1997.

[23] S. Van Huffel and P. Lemmerling, eds., *Total Least Squares and Errors-in-Variables Modeling: Analysis, Algorithms and Applications*, Kluwer Academic, Dordrecht, The Netherlands, 2002.

[24] S. Van Huffel and J. Vandewalle, *Analysis and properties of the generalized total least squares problem $AX \approx B$ when some or all columns in $A$ are subject to error*, SIAM J. Matrix Anal. Appl., 10 (1989), pp. 294–315.

[25] S. Van Huffel and J. Vandewalle, *The Total Least Squares Problem: Computational Aspects and Analysis*, SIAM, Philadelphia, 1991.

[26] P. Van Overschee and B. De Moor, *Subspace Identification for Linear Systems: Theory, Implementation, Applications*, Kluwer Academic, Dordrecht, The Netherlands, 1996.