On Weighted Structured Total Least Squares

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Abstract. In this contribution we extend our previous results on the structured total least squares problem to the case of weighted cost functions. It is shown that the computational complexity of the proposed algorithm is preserved linear in the sample size when the weight matrix is banded with bandwidth that is independent of the sample size.

1 Introduction

The *total least squares (TLS)* method (Golub and Van Loan, [1], Van Huffel and Vandewalle, [2])

$$\min_{\Delta A, \Delta B, X} \left\| \begin{bmatrix} \Delta A \; \Delta B \end{bmatrix} \right\|_{\mathrm{F}}^2 \quad \text{subject to} \quad (A - \Delta A)X = B - \Delta B \;, \tag{1}$$

is a solution technique for an overdetermined system of equations $AX \approx B$, $A \in \mathbb{R}^{m \times n}$, $B \in \mathbb{R}^{m \times d}$. It is a natural generalization of the least squares approximation method when the data in both A and B is perturbed. The method has been generalized in two directions:

– *weighted total least squares*

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

where $\|\Delta C\|_W^2 := \operatorname{vec}^\top(\Delta C^\top) W \operatorname{vec}(\Delta C^\top)$, $W > 0$, and
– *structured total least squares (STLS)*

$$\begin{aligned} \min_{\Delta A, \Delta B, X} \left\| \begin{bmatrix} \Delta A \; \Delta B \end{bmatrix} \right\|_{\mathrm{F}}^2 \quad &\text{subject to} \quad (A - \Delta A)X = B - \Delta B \quad \text{and} \\ &\begin{bmatrix} \Delta A \; \Delta B \end{bmatrix} \text{ has the same structure as } \begin{bmatrix} A \; B \end{bmatrix} \;. \end{aligned} \tag{3}$$

While the basic TLS problem allows for an analytic solution in terms of the singular value decomposition of the data matrix $C := \begin{bmatrix} A \; B \end{bmatrix}$, the weighted and structured TLS problems are solved numerically via local optimization methods.

In [4] we show that under a general assumption (see Assumption 1) about the structure, the cost function and first derivative of the STLS problem can be evaluated in $O(m)$ floating point operations (flops). This allows for efficient

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computational algorithms based on standard methods for local optimization. Via a similar approach, see (Markovsky et al., [5]), the weighted TLS problem can be solved efficiently when the weight matrix W is block-diagonal with blocks of size $n + d$.

In this paper, we extend our earlier results on the STLS problem by accounting for weighted cost function. Thus the weighted TLS problem becomes a special case of the considered weighted STLS problem when the data matrix is unstructured. In Sect. 2 we review the results of Markovsky, Van Huffel, Pintelon [4]. Section 3 presents the necessary modifications for the weighted STLS problem and Sect. 4 discusses the implementation of the algorithm.

2 Review of Results for the STLS Problem

Let $\mathcal{S} : \mathbb{R}^{n_p} \to \mathbb{R}^{m\times(n+d)}$ be an injective function. A matrix $C \in \mathbb{R}^{m\times(n+d)}$ is said to be $\mathcal{S}$-structured if $C \in \text{image}(\mathcal{S})$. The vector p for which $C = \mathcal{S}(p)$ is called the parameter vector of the structured matrix C. Respectively, $\mathbb{R}^{n_p}$ is called the parameter space of the structure $\mathcal{S}$. The aim of the STLS problem is to perturb as little as possible a given parameter vector p by a vector Δp, so that the perturbed structured matrix $\mathcal{S}(p + \Delta p)$ becomes rank deficient with rank at most n.

Problem 1 (STLS). Given a data vector $p \in \mathbb{R}^{n_p}$, a structure specification $\mathcal{S} : \mathbb{R}^{n_p} \to \mathbb{R}^{m\times(n+d)}$, and a rank specification n, solve the optimization problem

$$\hat{X} = \arg\min_{X,\Delta p} \|\Delta p\|_2^2 \quad \text{subject to} \quad \mathcal{S}(p - \Delta p)\begin{bmatrix} X \\ -I_d \end{bmatrix} = 0 \ . \tag{4}$$

Let $\begin{bmatrix} A \ B \end{bmatrix} := \mathcal{S}(p)$. Problem 1 makes precise the STLS problem formulation (3) from the introduction. In what follows, we often use the notation

$$X_{\text{ext}} := \begin{bmatrix} X \\ -I \end{bmatrix} .$$

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

$$\mathcal{S}(p) = S_0 + \sum_{i=1}^{n_p} S_i p_i, \quad \text{for all } p \in \mathbb{R}^{n_p} \text{ and for some } S_i,\ i = 1, \ldots, n_p \ . \tag{5}$$

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

Lemma 1. *Let $\mathcal{S} : \mathbb{R}^{n_p} \to \mathbb{R}^{m\times(n+d)}$ be an affine function. Then*

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

where

$$G(X) := \begin{bmatrix} \text{vec}\big((S_1 X_{\text{ext}})^\top\big) & \cdots & \text{vec}\big((S_{n_p} X_{\text{ext}})^\top\big) \end{bmatrix} \in \mathbb{R}^{md\times n_p} \ , \tag{6}$$

and

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

Using Lemma 1, we rewrite the affine STLS problem as follows

$$\min_X \Big(\min_{\Delta p} \|\Delta p\|_2^2 \quad \text{subject to} \quad G(X)\Delta p = r(X) \Big) \ . \tag{7}$$

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

Theorem 1 (Equivalent optimization problem for affine STLS). *Assuming that $n_p \geq md$, the affine STLS problem (7) is equivalent to*

$$\min_X f(X) \quad \textit{where} \quad f(X) := r^\top(X)\Gamma^\dagger(X)r(X) \quad \textit{and} \quad \Gamma(X) := G(X)G^\top(X) \ .$$

The significance of Theorem 1 is that the constraint and the decision variable Δp in problem (7) 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 (1) 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 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 $O(m^3)$ 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 $\Gamma(X)$ has a block-Toeplitz and block-banded structure, which can be exploited for efficient cost function and first derivative evaluations.

Assumption 1 (Flexible structure specification). *The structure specification $\mathcal{S} : \mathbb{R}^{n_p} \to \mathbb{R}^{m\times(n+d)}$ is such that for all $p \in \mathbb{R}^{n_p}$, the data matrix $\mathcal{S}(p) =: C =: \begin{bmatrix} A & B \end{bmatrix}$ is of the type*

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

Assumption 1 says that $\mathcal{S}(p)$ is composed of blocks, each one of which is block-Toeplitz, block-Hankel, unstructured, or exact. 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 1 is the essential structural assumption that we impose on the STLS problem. It is fairly general and covers many applications.

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

Theorem 2 (Structure of the weight matrix Γ). *Consider the equivalent optimization problem (1) from Theorem 1. If in addition to the assumptions of*

Theorem 1, the structure $\mathcal{S}$ is such that Assumption 1 holds, then the weight matrix $\Gamma(X)$ has the block-Toeplitz and block-banded structure,

$$\Gamma(X) = \begin{bmatrix} \Gamma_0 & \Gamma_1^\top & \cdots & \Gamma_s^\top & & \mathbf{0} \\ \Gamma_1 & \ddots & \ddots & \ddots & \ddots & \\ \vdots & \ddots & \ddots & \ddots & \ddots & \Gamma_s^\top \\ \Gamma_s & \ddots & \ddots & \ddots & \ddots & \vdots \\ & \ddots & \ddots & \ddots & \ddots & \Gamma_1^\top \\ \mathbf{0} & & \Gamma_s & \cdots & \Gamma_1 & \Gamma_0 \end{bmatrix} \in \mathbb{R}^{md \times md} \ , \qquad (8)$$

where $\Gamma_k \in \mathbb{R}^{dK \times dK}$, for $k = 0, 1, \dots, s$, and $s = \max_{l=1,\dots,q}(\mathbf{n}_l - 1)$.

3 Modifications for the Weighted STLS Problem

Next we consider the generalization of the STLS problem where the cost function is weighted.

Problem 2 (Weighted STLS). Given a data vector $p \in \mathbb{R}^{n_p}$, a positive definite weight matrix $W \in \mathbb{R}^{n_p \times n_p}$, a structure specification $\mathcal{S} : \mathbb{R}^{n_p} \to \mathbb{R}^{m \times (n+d)}$, and a rank specification n, solve the optimization problem

$$\hat{X}_{\mathrm{w}} = \arg\min_{X, \Delta p} \Delta p^\top W \Delta p \ \text{ subject to } \ \mathcal{S}(p - \Delta p) \begin{bmatrix} X \\ -I_d \end{bmatrix} = 0 \ . \qquad (9)$$

The counterpart of Theorem 1 for the case at hand is the following one.

Theorem 3 (Equivalent optimization problem for weighted STLS). *Assuming that $n_p \geq md$, the affine weighted STLS problem (9) is equivalent to*

$$\min_X f_{\mathrm{w}}(X) \quad \textit{where} \quad f_{\mathrm{w}}(X) := r^\top(X) \Gamma_{\mathrm{w}}^\dagger(X) r(X)$$
$$\textit{and} \quad \Gamma_{\mathrm{w}}(X) := G(X) W^{-1} G^\top(X) \ . \qquad (10)$$

Proof. The equivalent optimization problem in Theorem 1 is obtained by solving a least squares problem. In the weighted STLS case, we solve the weighted least squares problem

$$\min_{\Delta p} \Delta p^\top W \Delta p \quad \text{subject to} \quad G(X)\Delta p = r(X) \ .$$

The optimal parameter correction as a function of X is

$$\Delta p_{\mathrm{w}}(X) = W^{-1} G^\top(X) \big(G(X) W^{-1} G^\top(X) \big)^\dagger r(X) \ ,$$

so that

$$f_{\mathrm{w}}(X) = \Delta p_{\mathrm{w}}^\top(X) W \Delta p_{\mathrm{w}}(X) = r^\top(X) \big(\underbrace{G(X) W^{-1} G^\top(X)}_{\Gamma_{\mathrm{w}}} \big)^\dagger r(X) \ . \quad \square$$

In general neither the block-Toeplitz nor the block-banded properties of $\Gamma = GG^\top$ are present in $\Gamma_\mathrm{w} = GW^{-1}G^\top$. In the rest of this section, we show that in certain special cases these properties are preserved.

Assumption 2 (Block-diagonal weight matrix). *Consider the flexible structure specification of Assumption 1, let the blocks C^l, $l = 1, \dots, q$ be parameterized by parameter vectors $p_l \in \mathbb{R}^{n_{p,l}}$, and assume without loss of generality that $p = \mathrm{col}(p_1, \dots, p_q)$. The weight matrix W is assumed to be block-diagonal*

$$W = \mathrm{blk\,diag}(W^1, \dots, W^q), \qquad \textit{where} \quad W^l \in \mathbb{R}^{n_{p,l} \times n_{p,l}} \ .$$

Assumption 2 forbids cross-weighting among the parameters of the blocks $C^1, \dots, C^q$. Under Assumption 2 the effect of C^l on Γ_w is independent from those of the other blocks. Thus the problem of determining the structure of Γ_w, resulting from the flexible structure specification of C decouples into three independent problems: what is the structure of Γ_w, resulting from respectively an unstructured matrix C, a block-Hankel matrix C, and a block-Toeplitz matrix C.

In what follows "i-block-Toeplitz matrix" stands for block-Toeplitz matrix with $i \times i$ block size and "s-block-banded matrix" stands for a block-symmetric and block-banded matrix with upper/lower block-bandwidth i. Let $V := W^{-1}$ and $V_i := W_i^{-1}$.

Proposition 1. *Let G be defined as in (6) and let Assumptions 1 and 2 hold. If all blocks V^l corresponding to unstructured blocks C^l are $(n+d)K$-block-Toeplitz and all blocks V^l corresponding to block-Toeplitz/Hankel blocks C^l are dK-block-Toeplitz, $\Gamma_\mathrm{w} = GVG^\top$ is dK-block-Toeplitz.*

Proof. See the Appendix. □

For a particular type of weight matrices, the block-Toeplitz structure of Γ is preserved. More important, however, is the implication of the following proposition.

Proposition 2. *Let G be defined as in (6) and let Assumptions 1 and 2 hold. If W is p-block-banded, then $\Gamma_\mathrm{w} = GVG^\top$ is $(s+p)$-block-banded, where s is given in Theorem 2.*

Proof. See the Appendix. □

For block-banded weight matrix W, the block-banded structure of Γ is preserved, however, the block-bandwidth is increased by the block-bandwidth of W. In the following section, the block-banded structure of Γ (and Γ_w) is utilized for $O(m)$ cost function and first derivative evaluation.

Summary: We have established the following special cases:

V block-Toeplitz $\Longrightarrow \Gamma_\mathrm{w}$ block-Toeplitz (generally not block-banded),
V^l p-block-banded $\Longrightarrow \Gamma_\mathrm{w}$ $(s+p)$-block-banded (generally not block-Toeplitz),
W block-diagonal $\Longrightarrow \Gamma_\mathrm{w}$ s-block-banded (generally not block-Toeplitz).

The case W block-diagonal, i.e., $W^l = \mathrm{blk\,diag}(W_1^l, \dots, W_m^l)$, for $l = 1, \dots, q$, covers most applications of interest and will be considered in the next section.

4 Algorithm for Solving Weighted STLS Problem

In [3] we have proposed an algorithm for solving the STLS problem (4) with the flexible structure specification of Assumption 1. The structure of $\mathcal{S}(\cdot)$ is specified by the integer K, the number of rows in a block of a block-Toeplitz/Hankel structured block C^l, and the array $\mathtt{S} \in (\{\mathtt{T},\mathtt{H},\mathtt{U},\mathtt{E}\} \times \mathbb{N} \times \mathbb{N})^q$ that describes the structure of the blocks $\{C^l\}_{l=1}^q$. The lth element $\mathtt{S}_l$ of the array $\mathtt{S}$ specifies the block C^l by giving its type $\mathtt{S}_l(1)$, the number of columns $n_l = \mathtt{S}_l(2)$, and (if C^l is block-Hankel or block-Toeplitz) the column dimension $t_l = \mathtt{S}_l(3)$ of a block in C^l. Therefore, the input data for the STLS problem is the data matrix $\mathcal{S}(p)$ (alternatively the parameter vector p) and the structure specification K and $\mathtt{S}$.

It is shown that the blocks Γ_k of Γ are quadratic functions of X

$$\Gamma_k(X) = (I_K \otimes X_{\text{ext}}^\top) S_k (I_K \otimes X_{\text{ext}}^\top)^\top \;, \quad k = 0, 1, \dots, s \;, \tag{11}$$

where the matrices $S_k \in \mathbb{R}^{K(n+d)\times K(n+d)}$ depend on the structure $\mathcal{S}$. The first step of the algorithm is to translate the structure specification $\mathtt{S}$ to the set of matrices S_k, $k = 0, 1, \dots, s$. Then for a given X, the Γ_k matrices can be formed, which specifies the Γ matrix.

For cost function evaluation, the structured system of equations $\Gamma(X)y(X) = r(X)$ is solved and the product $f(X) = r^\top(X)y(X)$ is computed. Efficiency is achieved by exploiting the structure of Γ in solving the system of equations. Moreover, as shown in [3], the first derivative $f'(X)$ can also be evaluated from $y(X)$ with $O(m)$ extra computations. The resulting solution method is outlined in Algorithm 1.

Algorithm 1. Algorithm for solving the STLS problem

Input: structure specification $K, \mathtt{S}$ and matrices A and B, such that $\begin{bmatrix} A & B \end{bmatrix} = \mathcal{S}(p)$.
1: Form the matrices $\{S_k\}$.
2: Compute the TLS solution X_{ini} of $AX \approx B$.
3: Execute a standard optimization algorithm, e.g., the BFGS quasi-Newton method, for the minimization of f_0 over X with initial approximation X_{ini} and with efficient cost function and first derivative evaluation.
Output: $\hat{X}$ the approximation found by the optimization algorithm upon convergence.

The changes for the case of weighted STLS problem are only in (11). Now the matrix Γ is replaced by Γ_{w}, which is no longer block-Toeplitz but is s-block-banded with block-elements

$$\Gamma_{ij}(X) = (I_K \otimes X_{\text{ext}}^\top) S_{ij} (I_K \otimes X_{\text{ext}}^\top)^\top \;, \tag{12}$$

where

$$S_{ij} := \begin{cases} \operatorname{blk\,diag}(V_i^1, \dots, V_i^q) S_{i-j} & \text{if } 0 \le i-j \le s \\ S_{ji}^\top & \text{if } -s \le i-j < 0 \;. \\ 0 & \text{otherwise} \end{cases}$$

For an exact block C^l, with some abuse of notation, we define $W_i^l = 0$ for all i. (Our previous definition of W^l is an empty matrix since $p_l = 0$ in this case.)

5 Conclusions

We have extended the theory of Markovsky, Van Huffel, Pintelon ([4]) for the case of weighted STLS problems. The main question of interest is what properties of the Γ matrix in the equivalent optimization problem are preserved when the cost function is weighted. Block-Toeplitz inverse weight matrix V, results in corresponding Γ_{w} matrix that is also block-Toeplitz. More important for fast computational methods, however, is the fact that block-banded weight matrix W with block-bandwidth p leads to increase of the block-bandwidth of Γ with p. In particular W block-diagonal, results in Γ_{w} block-banded with the same bandwidth as Γ. This observation was used for efficient solution of weighted STLS problems.

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A Proof of Propositions 1 and 2

The G matrix, see (6), has the following structure $G = \begin{bmatrix} G^1 & \cdots & G^q \end{bmatrix}$, where $G^l \in \mathbb{R}^{md \times p_l}$ depends only on the structure of C^l (see Lemma 3.2 of [4]). For an unstructured block C^l,

$$G^l = I_m \otimes X_{\text{ext},l}^\top \ , \tag{13}$$

where $X_{\text{ext}} =: \text{col}(X_{\text{ext},1}, \ldots, X_{\text{ext},q})$, $X_{\text{ext},l} \in \mathbb{R}^{n_l \times d}$ and $\otimes$ is the Kronecker product. For a block-Toeplitz block C^l,

$$G^l = \begin{bmatrix} \mathbf{X}_1 & \mathbf{X}_2 & \cdots & \mathbf{X}_{\mathsf{n}_l} & 0 & \cdots & 0 \\ 0 & \mathbf{X}_1 & \mathbf{X}_2 & \cdots & \mathbf{X}_{\mathsf{n}_l} & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & & \ddots & 0 \\ 0 & \cdots & 0 & \mathbf{X}_1 & \mathbf{X}_2 & \cdots & \mathbf{X}_{\mathsf{n}_l} \end{bmatrix} \ , \tag{14}$$

where $\mathbf{X}_k := I_K \otimes X_{\text{ext},k}$, and for a block-Hankel block C^l,

$$G^l = \begin{bmatrix} \mathbf{X}_{\mathsf{n}_l} & \mathbf{X}_{\mathsf{n}_l - 1} & \cdots & \mathbf{X}_1 & 0 & \cdots & 0 \\ 0 & \mathbf{X}_{\mathsf{n}_l} & \mathbf{X}_{\mathsf{n}_l - 1} & \cdots & \mathbf{X}_1 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & & \ddots & 0 \\ 0 & \cdots & 0 & \mathbf{X}_{\mathsf{n}_l} & \mathbf{X}_{\mathsf{n}_l - 1} & \cdots & \mathbf{X}_1 \end{bmatrix} \ . \tag{15}$$

Due to Assumption 2, we have

$$\Gamma_{\mathrm{w}} = G V G^\top = \sum_{l=1}^{q} \underbrace{G^l V^l (G^l)^\top}_{\Gamma_{\mathrm{w}}^l} \ , \tag{16}$$

so that we need to consider the three independent problems: structure of Γ_{w}^l for respectively unstructured, block-Toeplitz, and block-Hankel block C^l. The statements of Propositions 1 and 2 are now easy to see by substituting respectively (13), (14), and (15) in (16) and doing the matrix products.