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THE TOTAL LEAST SQUARES PROBLEM IN $AX \approx B$. A NEW CLASSIFICATION WITH THE RELATIONSHIP TO THE CLASSICAL WORKS*

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Abstract. The presented paper revisits the analysis of the total least squares (TLS) problem $AX \approx B$ with multiple right-hand sides given by Sabine Van Huffel and Joos Vandewalle, in the monograph: The Total Least Squares Problem: Computational Aspects and Analysis, SIAM Publications, Philadelphia 1991.

The newly proposed classification is based on properties of the singular value decomposition of the extended matrix $[B|A]$. It aims at identifying the cases when a TLS solution does or does not exist, and when the output computed by the classical TLS algorithm, given by Van Huffel and Vandewalle, is actually a TLS solution. The presented results on existence and uniqueness of the TLS solution reveal subtleties that were not captured in the known literature.

Key words. total least squares (TLS), multiple right-hand sides, linear approximation problems, orthogonally invariant problems, orthogonal regression, errors-in-variables modeling.

AMS subject classifications. 15A24, 15A60, 65F20, 65F30.

1. Introduction. This paper focuses on the *total least squares (TLS)* formulation of the linear approximation problem with *multiple right-hand sides*

$$AX \approx B, \qquad A \in \mathbb{R}^{m\times n}, \quad X \in \mathbb{R}^{n\times d}, \quad B \in \mathbb{R}^{m\times d}, \quad A^T B \neq 0, \tag{1.1}$$

or, equivalently,

$$\left[\begin{array}{c|c} B & A \end{array}\right] \left[\begin{array}{c} -I_d \\ \hline X \end{array}\right] \approx 0. \tag{1.2}$$

We concentrate on the *incompatible problem* (1.1), i.e. $\mathcal{R}(B) \not\subset \mathcal{R}(A)$. The compatible case reduces to finding a solution of a system of linear algebraic equations. In TLS, contrary to the ordinary least squares, the correction is allowed to compensate for errors in the *system (data) matrix* A as well as in the *right-hand side (observation) matrix* B, and the matrices E and G are sought to minimize the Frobenius norm in

$$\min_{X,E,G} \left\| \left[\begin{array}{c|c} G & E \end{array}\right] \right\|_F \qquad \text{subject to} \qquad (A+E)X = B+G. \tag{1.3}$$

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Throughout the whole paper, *any* matrix X which solves the corrected system in (1.3) is called a *TLS solution*. Similarly to the ordinary least squares, we are often interested in TLS solutions *minimal in the 2-norm and/or in the Frobenius norm*.

Mathematically equivalent problems have been independently investigated in several areas as *orthogonal regression* and *errors-in-variables modeling*, see [18, 19]. It is worth noting that other norms than the Frobenius norm in (1.3) can also be relevant in practice, see, e.g., [20].

The TLS problem (1.1)–(1.3) has been investigated in its algebraic setting for decades, see the early works [6], [4, Section 6], [14]. In [7] it is shown that even with $d = 1$ (which gives $Ax \approx b$, where b is an m-vector) the TLS problem may not have a solution and, when the solution exists, it may not be unique; see also [5, pp. 324–326]. The classical book [17] introduces the *generic–nongeneric* terminology representing the basic classification of TLS problems. If $d = 1$, then the *generic problems* simply represent problems that have a (possibly nonunique) solution, whereas *nongeneric problems* do not have a solution in the sense of (1.3). This is no longer true for multiple right-hand sides, where $d > 1$. The monograph [17] analyzes only two particular cases characterized by the special distribution of singular values of the extended matrix $[B|A]$. The so called *classical TLS algorithm* presented in [17], however, for *any* A, B computes some output X. The relationship of this output to the original problem is not always clear.

For $d = 1$, the TLS problem does not have a solution when the *collinearities among columns of A are stronger than the collinearities between $\mathcal{R}(A)$ and b*; see [9, 10, 11] for a recent description. An analogous situation may occur for $d > 1$, but here the difficulty can be caused for *different columns of B by different subsets of columns of A*. Therefore it is no longer possible to stay with the generic–nongeneric classification of TLS problems. This is also the reason why the question remained open in [17]. In this paper we try to fill this gap and investigate existence and uniqueness of the TLS solution with $d > 1$ in full generality.

The organization of this paper is as follows. Section 2 recalls some basic results. Section 3 introduces *problems of what we call the 1st class*. After recalling known results for two special distributions of singular values in Sections 3.1 and 3.2, we turn to the general case in Section 3.3. The new classification is introduced in Section 4. Section 5 introduces *problems of the 2nd class*. Section 6 links the new classification with the *classical TLS algorithm* from [17] and Section 7 concludes the paper.

2. Preliminaries. As usual, $\sigma_j(M)$ denotes the jth largest singular value, $\mathcal{R}(M)$ and $\mathcal{N}(M)$ the range and the null space, $\|M\|_F$ and $\|M\|$ the Frobenius norm and the 2-norm of the given matrix M, respectively, and $M^\dagger$ denotes the Moore-Penrose pseudoinverse of M. Further, $\|v\|$ denotes the 2-norm of the given vector v, $I_k \in \mathbb{R}^{k\times k}$ denotes the k-by-k identity matrix.

In order to simplify the notation we assume, with no loss of generality, $m \geq n+d$ (otherwise, we can simply add zero rows). Consider the SVD of A, $r \equiv \operatorname{rank}(A)$,

$$A = U'\Sigma'(V')^T, \tag{2.1}$$

where $(U')^{-1} = (U')^T$, $(V')^{-1} = (V')^T$, $\Sigma' = \operatorname{diag}(\sigma'_1, \ldots, \sigma'_r, 0) \in \mathbb{R}^{m\times n}$, and

$$\sigma'_1 \geq \ldots \geq \sigma'_r > \sigma'_{r+1} = \ldots = \sigma'_n \equiv 0. \tag{2.2}$$

Similarly, consider the SVD of $[B|A]$, $s \equiv \operatorname{rank}([B|A])$,

$$\left[\; B \;\middle|\; A \;\right] = U\Sigma V^T, \tag{2.3}$$

where $U^{-1} = U^T$, $V^{-1} = V^T$, $\Sigma = \mathrm{diag}(\sigma_1, \ldots, \sigma_s, 0) \in \mathbb{R}^{m\times(n+d)}$, and

$$\sigma_1 \geq \ldots \geq \sigma_s > \sigma_{s+1} = \ldots = \sigma_{n+d} \equiv 0. \tag{2.4}$$

If $s = n+d$ (which implies $r = n$), then Σ' and Σ have no zero singular values. Among the singular values, a key role is played by σ_{n+1}, where n represents the number of columns of A. In order to handle possible higher multiplicity of σ_{n+1}, we introduce the following notation

$$\sigma_p \equiv \sigma_{n-q} > \underbrace{\sigma_{n-q+1} = \ldots = \sigma_n}_{q} = \underbrace{\sigma_{n+1} = \ldots = \sigma_{n+e}}_{e} > \sigma_{n+e+1}, \tag{2.5}$$

where q singular values to the left and $e-1$ singular values to the right are equal to σ_{n+1}, and hence $q \geq 0$, $e \geq 1$. For convenience we denote $n - q \equiv p$. (Clearly $\sigma_p \equiv \sigma_{n-q}$ is not defined iff $q = n$, similarly σ_{n+e+1} is not defined iff $e = d$.)

For an integer Δ (not necessarily nonnegative) it will be useful to consider the following partitioning

$$\Sigma = \begin{array}{c} \overbrace{\hphantom{\Sigma_1^{(\Delta)}}}^{n-\Delta}\overbrace{\hphantom{\Sigma_2^{(\Delta)}}}^{d+\Delta} \\ \left[\begin{array}{c|c} \Sigma_1^{(\Delta)} & \Sigma_2^{(\Delta)} \end{array}\right] \end{array} \Big\} m, \qquad V = \begin{array}{c} \overbrace{\hphantom{V_{11}^{(\Delta)}}}^{n-\Delta}\overbrace{\hphantom{V_{12}^{(\Delta)}}}^{d+\Delta} \\ \left[\begin{array}{c|c} V_{11}^{(\Delta)} & V_{12}^{(\Delta)} \\ \hline V_{21}^{(\Delta)} & V_{22}^{(\Delta)} \end{array}\right] \end{array} \begin{array}{l} \}\, d \\ \}\, n \end{array}, \tag{2.6}$$

where $\Sigma_1^{(\Delta)} \in \mathbb{R}^{m\times(n-\Delta)}$, $\Sigma_2^{(\Delta)} \in \mathbb{R}^{m\times(d+\Delta)}$, and $V_{11}^{(\Delta)} \in \mathbb{R}^{d\times(n-\Delta)}$, $V_{12}^{(\Delta)} \in \mathbb{R}^{d\times(d+\Delta)}$, $V_{21}^{(\Delta)} \in \mathbb{R}^{n\times(n-\Delta)}$, $V_{22}^{(\Delta)} \in \mathbb{R}^{n\times(d+\Delta)}$. When $\Delta = 0$, the partitioning conforms to the fact that $[B|A]$ is created by A appended by the matrix B with d columns and in this case the upper index is omitted, $\Sigma_1 \equiv \Sigma_1^{(0)}$, etc.

The classical analysis of the TLS problem with a single right-hand side ($d = 1$) in [7], and the theory developed in [17] were based on relationships between the singular values of A and $[B|A]$. For $d = 1$, in particular, $\sigma'_n > \sigma_{n+1}$ represents a *sufficient (but not necessary) condition* for the existence and uniqueness of the solution. In order to extend this condition to the case $d > 1$, the following generalization of [7, Theorem 4.1] is useful.

Theorem 2.1. *Let (2.1) be the SVD of A and (2.3) the SVD of $[B|A]$ with the partitioning given by (2.6), $m \geq n + d$, $\Delta \geq 0$. If*

$$\sigma'_{n-\Delta} > \sigma_{n-\Delta+1}, \tag{2.7}$$

then $\sigma_{n-\Delta} > \sigma_{n-\Delta+1}$. Moreover, $V_{12}^{(\Delta)}$ is of full row rank equal to d, and $V_{21}^{(\Delta)}$ is of full column rank equal to $(n - \Delta)$.

The first part follows immediately from the interlacing theorem for singular values [17, Theorem 2.4, p. 32] (see also [13]). For the proof of the second part see [21, Lemma 2.1] or [17, Lemma 3.1, pp. 64–65]. (Please note the different ordering of the partitioning of V in [21, 17].)

We start our analysis with the following definition.

Definition 2.2 (Problems of the 1st class and of the 2nd class). *Consider a TLS problem (1.1)–(1.3), $m \geq n + d$. Let (2.3) be the SVD of $[B|A]$ with the partitioning given by (2.6). Take $\Delta \equiv q$, where q is the "left multiplicity" of σ_{n+1} given by (2.5).*

- *If $V_{12}^{(q)}$ is of full row rank d,*
  then we call (1.1)–(1.3) a TLS problem of the 1st class.
- *If $V_{12}^{(q)}$ is rank deficient (i.e. has linearly dependent rows),*
  then we call (1.1)–(1.3) a TLS problem of the 2st class.

The set of all problems of the 1st class will be denoted by $\mathscr{F}$. The set of all problems of the 2nd class will be denoted by $\mathscr{S}$.

3. Problems of the 1st class. For $d = 1$, the right singular vector subspace corresponding to the smallest singular value σ_{n+1} of $[b|A]$ contains for a TLS problem of the 1st class a singular vector with a nonzero first component. Consequently, the TLS problem has a (possibly nonunique) solution. As we will see, for $d > 1$ an analogous property does not hold. The TLS problem of the 1st class with $d > 1$ may not have a solution. First we recall known results for two special cases of problems of the 1st class.

3.1. Problems of the 1st class with unique TLS solution. Consider a TLS problem of the 1st class. Assume that $\sigma_n > \sigma_{n+1}$, i.e. $q = 0$ ($p = n$). Setting $\Delta \equiv q = 0$ in (2.6), $V_{12}^{(q)} \equiv V_{12}$ is a square (and nonsingular) matrix. Define the *correction matrix*

$$\left[\ G \mid E\ \right] \equiv -U \left[\ 0 \mid \Sigma_2\ \right] V^T = -U\,\Sigma_2 \left[\ V_{12}^T \mid V_{22}^T\ \right]. \tag{3.1}$$

Clearly, $\|[G|E]\|_F = (\sum_{j=n+1}^{n+d} \sigma_j^2)^{1/2}$, and the *corrected matrix* $[B+G|A+E]$ represents, by the Eckart-Young-Mirsky theorem [1, 8], the unique rank n approximation of $[B|A]$ with minimal $[G|E]$ in the Frobenius norm.

The columns of the matrix $[V_{12}^T|V_{22}^T]^T$ represent a basis for the null space of the corrected matrix $[B+G|A+E] \equiv U\Sigma_1[V_{11}^T|V_{21}^T]$. Since V_{12} is square and nonsingular,

$$\left[\ B+G \mid A+E\ \right] \left[\frac{-I_d}{-V_{22}V_{12}^{-1}} \right] = 0,$$

which gives the uniquely determined TLS solution

$$X_{\mathrm{TLS}} \equiv X^{(0)} \equiv -V_{22}V_{12}^{-1}. \tag{3.2}$$

We summarize these observations in the following theorem, see [17, Theorem 3.1, pp. 52–53].

THEOREM 3.1. *Consider a TLS problem of the 1st class. If*

$$\sigma_n > \sigma_{n+1}, \tag{3.3}$$

then with the partitioning of the SVD of $[B|A]$ given by (2.6), $\Delta \equiv q = 0$, $V_{12} \in \mathbb{R}^{d\times d}$ is square and nonsingular, and (3.2) represents the unique TLS solution of the problem (1.1)–(1.3) with the corresponding correction $[G|E]$ given by (3.1).

Theorem 2.1 gives the following corollary.

COROLLARY 3.2. *Let (2.1) be the SVD of A and (2.3) the SVD of $[B|A]$ with the partitioning given by (2.6), $m \geq n+d$, $\Delta \equiv 0$. If*

$$\sigma'_n > \sigma_{n+1}, \tag{3.4}$$

then (1.1)–(1.3) is a problem of the 1st class, $\sigma_n > \sigma_{n+1}$, and (3.2) represents the unique TLS solution of the problem (1.1)–(1.3) with the corresponding correction matrix $[G|E]$ given by (3.1).

We see that (3.4) represents a sufficient condition for the existence and uniqueness of the TLS solution of the problem (1.1)–(1.3). This condition is, however, intricate. It may look as the key to the analysis of the TLS problem, in particular when one considers the following corollary of the interlacing theorem for singular values and Theorem 2.1; see [17, Corollary 3.4, p. 65].

COROLLARY 3.3. *Let (2.1) be the SVD of A and (2.3) the SVD of $[B|A]$ with the partitioning given by (2.6), $m \geq n+d$, $\Delta \equiv q \geq 0$. Then the following conditions are equivalent:*

(i) $\sigma'_{n-q} > \sigma_{n-q+1} = \ldots = \sigma_{n+d}$,
(ii) $\sigma_{n-q} > \sigma_{n-q+1} = \ldots = \sigma_{n+d}$ *and* $V_{12}^{(q)}$ *is of (full row) rank d.*

In the following discussion we restrict ourselves to the *single right-hand side* case. The condition (i) implies that the TLS problem is of the 1st class. If $d = 1$ and $q = 0$, then (i) reduces to (3.4) and the statement of Corollary 3.3 says that $\sigma'_n > \sigma_{n+1}$ if and only if $\sigma_n > \sigma_{n+1}$ and $[1, 0, \ldots, 0]^T v_{n+1} \neq 0$. In order to show the difficulty and motivate the classification in the sequel, we now consider all remaining possibilities for the case $d = 1$. It should be, however, understood that they go beyond the problems of the 1st class and the unique TLS solution. If $\sigma'_n = \sigma_{n+1}$, then it may happen *either* $\sigma_n > \sigma_{n+1}$ and $i_1^T v_{n+1} = 0$, which means that the TLS problem is not of the 1st class and it does not have a solution, *or* $\sigma_n = \sigma_{n+1}$. In the latter case, depending on the relationship between σ'_{n-q} and $\sigma_{n-q+1} = \ldots = \sigma_{n+1}$ for some $q > 0$, see Corollary 3.3, the TLS problem may have a nonunique solution, if the TLS problem is of the 1st class (see the next section), or the solution may not exist. We see that an attempt to base the analysis on the relationship between σ'_n and σ_{n+1} becomes very involved.

The situation becomes more transparent with the use of the core problem concept from [11]. For any linear approximation problem $Ax \approx b$ (we still consider $d = 1$) there are orthogonal matrices P, R such that

$$P^T \left[\ b \mid A\ \right] \left[\begin{array}{c|c} 1 & 0 \\ \hline 0 & R \end{array}\right] = \left[\begin{array}{c||c|c} b_1 & A_{11} & 0 \\ \hline 0 & 0 & A_{22} \end{array}\right], \tag{3.5}$$

where:

(i) A_{11} is of minimal dimensions and A_{22} is of maximal dimensions (A_{22} may also have zero number of rows and/or columns) over all orthogonal transformations of $[b|A]$ yielding the structure (3.5) of zero and nonzero blocks. Suppose $b \not\perp \mathcal{R}(A)$ has nonzero projections on exactly ℓ left singular vector subspaces of A corresponding to distinct (nonzero) singular values. Then among all decompositions of the form (3.5) the minimally dimensioned A_{11} is $\ell \times \ell$ if $Ax \approx b$ is compatible, and $(\ell+1) \times \ell$ if $Ax \approx b$ is incompatible (see [11, Theorem 2.2]).
(ii) All singular values of A_{11} are simple and nonzero, all singular values of $[b_1|A_{11}]$ are simple and, since $b \notin \mathcal{R}(A)$, nonzero (recall that we consider only the incompatible problems),
(iii) first components of all right singular vectors of $[b_1|A_{11}]$ are nonzero,
(iv) $\sigma_{\min}(A_{11}) > \sigma_{\min}([b_1|A_{11}])$. Moreover, singular values of A_{11} *strictly interlace* singular values of $[b_1|A_{11}]$,

see [11, Section 3]. The minimally dimensioned subproblem $A_{11}x_1 \approx b_1$ is then called the *core problem* within $Ax \approx b$. The SVD of the block structured matrix on the right-hand side in (3.5) can be obtained as a direct sum of the SVD decompositions of the blocks $[b_1|A_{11}]$ and A_{22}, just by extending the singular vectors corresponding to the first block by zeros on the bottom and the singular vectors corresponding to the second block by zeros on the top. Consequently, considering the special structure of the orthogonal transformation $\mathrm{diag}(1, R)$ in (3.5), which does not change the first components of the right singular vectors, all right singular vectors of $[b|A]$ with nonzero first components correspond to the block $[b_1|A_{11}]$, and all right singular vectors of $[b|A]$ with zero first component correspond to A_{22}. Moreover,

$$\begin{aligned} \sigma'_n \equiv \quad \sigma_{\min}(A) \quad &= \min\{\sigma_{\min}(A_{11}), \sigma_{\min}(A_{22})\}, \\ \sigma_{n+1} \equiv \sigma_{\min}([b|A]) &= \min\{\sigma_{\min}([b_1|A_{11}]), \sigma_{\min}(A_{22})\}. \end{aligned}$$

We will review all possible situations:

Case 1: $\sigma'_n > \sigma_{n+1}$. This happens if and only if $\sigma_{\min}(A_{22}) > \sigma_{\min}([b_1|A_{11}]) = \sigma_{n+1}$ which is equivalent to the existence of the unique TLS solution.

Case 2: $\sigma_{\min}(A_{22}) \equiv \sigma'_n = \sigma_{n+1}$. Here we have to distinguish two cases:

Case 2a: $\sigma_{\min}(A) = \sigma_{\min}([b|A]) = \sigma_{\min}([b_1|A_{11}])$. This guarantees the existence of the (minimum norm) TLS solution. All singular values of A equal to $\sigma_{\min}(A)$ are the singular values of the block A_{22}. Consequently, the multiplicity of $\sigma_{\min}([b|A])$ is larger by one than the multiplicity of $\sigma_{\min}(A)$.

Case 2b: $\sigma_{\min}(A) = \sigma_{\min}([b|A]) < \sigma_{\min}([b_1|A_{11}])$. Then the multiplicities of $\sigma_{\min}(A)$ and $\sigma_{\min}([b|A])$ are equal, all right singular vectors of $[b|A]$ corresponding to $\sigma_{\min}([b|A])$ have zero first components, and the TLS solution does not exist.

Summarizing, the TLS solution exists if and only if *either* $\sigma_{\min}(A) > \sigma_{\min}([b|A])$, *or* $\sigma_{\min}(A) = \sigma_{\min}([b|A])$ with different multiplicities for $\sigma_{\min}(A)$ and $\sigma_{\min}([b|A])$. In terms of the singular values of subblocks in the core reduction (3.5),

$$\begin{aligned} \sigma_{\min}(A_{22}) > \sigma_{\min}([b_1|A_{11}]) \quad &\Longleftrightarrow \quad \text{TLS solution exists and is unique,} \\ \sigma_{\min}(A_{22}) = \sigma_{\min}([b_1|A_{11}]) \quad &\Longleftrightarrow \quad \text{TLS solution exists and is not unique,} \\ \sigma_{\min}(A_{22}) < \sigma_{\min}([b_1|A_{11}]) \quad &\Longleftrightarrow \quad \text{TLS solution does not exist.} \end{aligned}$$

If the TLS solution exists, then the minimum norm TLS solution can always be computed, and it is automatically given by the core problem formulation. If the TLS solution does not exist, then the core problem formulation gives the solution equivalent to the minimum norm *nongeneric* solution constructed in [17].

We will see that in the multiple right-hand sides case the situation is much more complicated.

3.2. Problems of the 1st class with nonunique TLS solutions—a special case. Consider a TLS problem of the 1st class. Assume that $e \equiv d$ in (2.5), i.e. let all the singular values starting from $\sigma_{n-q+1} \equiv \sigma_{p+1}$ be equal,

$$\sigma_1 \geq \ldots \geq \sigma_p > \sigma_{p+1} = \ldots = \sigma_{n+1} = \ldots = \sigma_{n+d} \geq 0. \tag{3.6}$$

The case $q = 0$ ($p = n$) reduces to the problem with unique TLS solution discussed in Section 3.1. If $q = n$ ($p = 0$), i.e. $\sigma_1 = \ldots = \sigma_{n+d}$, then the columns of $[B|A]$ are mutually orthogonal and $[B|A]^T[B|A] = \sigma_1^2 I_{n+d}$. Then it seems meaningless to approximate B by the columns of A, and we will get consistently with [17] the trivial solution $X_{\mathrm{TLS}} \equiv 0$ (this case does not satisfy the nontriviality assumption $A^T B \neq 0$ in (1.1)). Therefore in this section the interesting case is represented by $n > q > 0$ ($0 < p < n$).

We first construct the solution minimal in norm. Since $V_{12}^{(q)} \in \mathbb{R}^{d\times(q+d)}$ is of full row rank, there exists an orthogonal matrix $Q \in \mathbb{R}^{(q+d)\times(q+d)}$ such that

$$\left[\begin{array}{c} V_{12}^{(q)} \\ \hline V_{22}^{(q)} \end{array}\right] Q \equiv \left[\begin{array}{c} v_{p+1}, \ldots, v_{n+d} \end{array}\right] Q = \left[\begin{array}{c|c} 0 & \Gamma \\ \hline Y & Z \end{array}\right], \tag{3.7}$$

where $\Gamma \in \mathbb{R}^{d\times d}$ is square and nonsingular. Such an orthogonal matrix Q can be obtained, e.g., using the LQ decomposition of $V_{12}^{(q)}$. Consider the partitioning $Q = [Q_1|Q_2]$, where $Q_2 \in \mathbb{R}^{(q+d)\times d}$ has d columns. Then the columns of Q_2 form an orthonormal basis of the subspace spanned by the columns of $V_{12}^{(q)T}$, $Q_1 \in \mathbb{R}^{(q+d)\times q}$ is an orthonormal basis of its orthogonal complement, and

$$\left[\begin{array}{c} \Gamma \\ \hline Z \end{array}\right] = \left[\begin{array}{c} V_{12}^{(q)} \\ \hline V_{22}^{(q)} \end{array}\right] Q_2, \qquad V_{12}^{(q)} = \Gamma Q_2^T. \tag{3.8}$$

Define the correction matrix

$$\begin{aligned} \left[\begin{array}{c|c} G & E \end{array}\right] &\equiv - \left[\begin{array}{c|c} B & A \end{array}\right] \left[\begin{array}{c} \Gamma \\ \hline Z \end{array}\right] \left[\begin{array}{c} \Gamma \\ \hline Z \end{array}\right]^T \\ &= -U\Sigma V^T \left[\begin{array}{c} V_{12}^{(q)} \\ \hline V_{22}^{(q)} \end{array}\right] Q_2 Q_2^T \left[\begin{array}{c} V_{12}^{(q)} \\ \hline V_{22}^{(q)} \end{array}\right]^T \\ &= -\sigma_{n+1} \left[\begin{array}{c} u_{p+1}, \ldots, u_{n+d} \end{array}\right] Q_2 Q_2^T \left[\begin{array}{c} v_{p+1}, \ldots, v_{n+d} \end{array}\right]^T, \end{aligned} \tag{3.9}$$

where u_j and v_j represent left and right singular vectors of the matrix $[B|A]$, respectively. If $\sigma_{p+1} = \ldots = \sigma_{n+d} = 0$, then the correction matrix is a zero matrix ($\sigma_{n+1} = 0$) and the problem is compatible, thus we consider $\sigma_{p+1} = \ldots = \sigma_{n+d} > 0$.

Note that with the choice of any other matrix $Q' = [Q_1'|Q_2']$ giving a decomposition of the form (3.7), Q_2' represents an orthonormal basis of the subspace spanned by the columns of $V_{12}^{(q)T}$, and therefore $Q_2' = Q_2\Psi$ for some orthogonal matrix $\Psi \in \mathbb{R}^{d\times d}$. Consequently, (3.9) is uniquely determined independently on the choice of Q in (3.7).

Clearly, $\|[G|E]\|_F = \sigma_{n+1}\|Q_2Q_2^T\|_F = \sigma_{n+1}\sqrt{d}$ and the corrected matrix

$$\left[\begin{array}{c|c} B+G & A+E \end{array}\right] \equiv \left[\begin{array}{c|c} B & A \end{array}\right] \left(I_{n+d} - \left[\begin{array}{c} \Gamma \\ \hline Z \end{array}\right] \left[\begin{array}{c} \Gamma \\ \hline Z \end{array}\right]^T \right)$$

represents the rank n approximation of $[B|A]$ such that the Frobenius norm of the correction matrix $[G|E]$ is minimal, by the Eckart-Young-Mirsky theorem.

The columns of the matrix $[\Gamma^T|Z^T]^T$ represent a basis for the null space of the corrected matrix $[B+G|A+E]$. Since Γ is square and nonsingular,

$$\left[\begin{array}{c|c} B+G & A+E \end{array}\right] \left[\begin{array}{c} -I_d \\ \hline -Z\Gamma^{-1} \end{array}\right] = 0,$$

which gives the TLS solution

$$X_{\mathrm{TLS}} \equiv -Z\Gamma^{-1} = -\left[\begin{array}{c|c} Y & Z \end{array}\right] Q^T Q \left[\begin{array}{c} 0 \\ \hline \Gamma^{-1} \end{array}\right] - V_{22}^{(q)} V_{12}^{(q)\dagger} \equiv X^{(q)}. \tag{3.10}$$

This can be expressed as

$$X_{\mathrm{TLS}} = \left(A^T A - \sigma_{n+1}^2 I_n\right)^{\dagger} A^T B,$$

see [17, Theorem 3.10, pp. 62–64]. The solution (3.10) and the correction (3.9) do not depend on the choice of the matrix Q in (3.7). We summarize these observations in the following theorem (see [17, Theorem 3.9, pp. 60–62]).

THEOREM 3.4. *Consider a TLS problem of the 1st class. Let (2.3) be the SVD of $[B|A]$ with the partitioning given by (2.6), $\Delta \equiv q < n$, $p \equiv n - q$. If*

$$\sigma_p > \sigma_{p+1} = \ldots = \sigma_{n+d}, \tag{3.11}$$

then (3.10) represents a TLS solution X_{TLS} of the problem (1.1)–(1.3). This is the unique solution of the minimal Frobenius norm and 2-norm, with the corresponding unique correction matrix $[G|E]$ given by (3.9).

Using Corollary 3.3 we get

$$\sigma'_p > \sigma_{p+1} = \ldots = \sigma_{n+d}, \tag{3.12}$$

which represents a sufficient condition for the existence of the TLS solution of the TLS problem (1.1)–(1.3) minimal in the Frobenius norm and the 2-norm.

The correction matrix minimal in the Frobenius norm can be in this special case constructed from *any* d vectors selected among $q+d$ columns $v_{p+1}, \ldots, v_{n+d}$ (or their orthogonal linear transformation) of the matrix V such that their top d-subvectors create a d-by-d square nonsingular matrix. The equality of the last $q+d$ singular values ensures that the Frobenius norm of the corresponding correction matrix is still equal to $\sigma_{n+1}\sqrt{d}$. It can be shown, that for any such choice a norm of the corresponding solution $\widetilde{X}$ is larger than or equal to the norm of $X^{(q)}$ given by (3.10), and any such $\widetilde{X}$ represents a TLS solution. Consequently, the special TLS problem satisfying (3.6) has infinitely many solutions.

3.3. Problems of the 1st class—the general case. Here we consider a TLS problem of the 1st class with a general distribution of singular values. We will discuss only the remaining cases not covered in the previous two sections, i.e., $n \geq q > 0$ ($0 \leq p < n$, recall that $p = n - q$) and $e < d$, giving

$$\sigma_1 \geq \ldots \geq \sigma_p > \sigma_{p+1} = \ldots = \sigma_{n+1} = \ldots = \sigma_{n+e} > \sigma_{n+e+1} \geq \ldots \geq \sigma_{n+d} \geq 0$$

(note that σ_p does not exist for $q = n$ ($p = 0$)). We will see that in this general case the problem (1.1)–(1.3) *may not have a solution.*

We try to construct a TLS solution with the same approach as in Section 3.2, and we will show that it may fail. Since, with the partitioning (2.6), $\Delta \equiv q$, the matrix $V_{12}^{(q)} \in \mathbb{R}^{d\times(q+d)}$ is of full row rank, there exists an orthogonal matrix $Q \in \mathbb{R}^{(q+d)\times(q+d)}$ such that

$$\left[\begin{array}{c} V_{12}^{(q)} \\ \hline V_{22}^{(q)} \end{array}\right] Q \equiv \left[\begin{array}{c} v_{p+1}, \ldots, v_{n+d} \end{array}\right] Q = \left[\begin{array}{c|c} 0 & \Gamma \\ \hline Y & Z \end{array}\right], \tag{3.13}$$

where $\Gamma \in \mathbb{R}^{d\times d}$ is square and nonsingular. With the partitioning $Q = [Q_1|Q_2]$, where $Q_1 \in \mathbb{R}^{(q+d)\times q}$, $Q_2 \in \mathbb{R}^{(q+d)\times d}$, the columns of Q_2 form an orthonormal basis of the subspace spanned by the columns of $V_{12}^{(q)T}$, and

$$\left[\frac{\Gamma}{Z}\right] = \left[\frac{V_{12}^{(q)}}{V_{22}^{(q)}}\right] Q_2, \qquad V_{12}^{(q)} = \Gamma Q_2^T. \tag{3.14}$$

Following [17], it is tempting to define the correction matrix

$$\begin{aligned}
[\; G \mid E \;] &\equiv -[\; B \mid A \;] \left[\frac{\Gamma}{Z}\right] \left[\frac{\Gamma}{Z}\right]^T \qquad (3.15)\\
&= -U\Sigma V^T \left[\frac{V_{12}^{(q)}}{V_{22}^{(q)}}\right] Q_2 Q_2^T \left[\frac{V_{12}^{(q)}}{V_{22}^{(q)}}\right]^T \\
&= -[\; u_{p+1}, \ldots, u_{n+d} \;] \operatorname{diag}(\sigma_{p+1}, \ldots, \sigma_{n+d}) Q_2 Q_2^T [\; v_{p+1}, \ldots, v_{n+d} \;]^T,
\end{aligned}$$

which differs from (3.9) because the diagonal factor is no longer a scalar multiple of the identity matrix. Analogously to the previous section, the matrix (3.15) is uniquely determined independently on the choice of Q in (3.13).

The columns of the matrix $[\Gamma^T|Z^T]^T$ are in the null space of the corrected matrix

$$[\; B+G \mid A+E \;] \equiv [\; B \mid A \;] \left(I_{n+d} - \left[\frac{\Gamma}{Z}\right] \left[\frac{\Gamma}{Z}\right]^T \right). \tag{3.16}$$

In general the columns of $[\Gamma^T|Z^T]^T$ do not represent *a basis* for the null space of the corrected matrix. If A is not of full column rank, the extended matrix $[B|A]$ has a zero singular value with the corresponding right singular vector having the first d entries equal to zero. Such a right singular vector is in the null space of the corrected matrix but it can not be obtained as a linear combination of the columns of $[\Gamma^T|Z^T]^T$. Since Γ is square and nonsingular,

$$[\; B+G \mid A+E \;] \left[\frac{-I_d}{-Z\Gamma^{-1}}\right] = 0,$$

and we can construct

$$X^{(q)} \equiv -Z\Gamma^{-1} = -V_{22}^{(q)} V_{12}^{(q)\dagger}. \tag{3.17}$$

The matrices (3.17) and (3.15) do not depend on the choice of Q in (3.13). The matrix $X^{(q)}$ given by (3.17) is a natural generalization of $X^{(q)}$ given by (3.10). The *classical TLS algorithm* [15, 16] (see also [17]) applied to a TLS problem of the 1st class returns as output the matrix $X^{(q)}$ given by (3.17) with the matrices G, E given by (3.15). We will show, however, that $X^{(q)}$ is not necessarily a TLS solution.

We first focus on the question whether there exists another correction $\widetilde{E}$, $\widetilde{G}$ corresponding to the last $q+d$ columns of V that makes the corrected system compatible. Such a correction can be constructed analogously to (3.13) by considering an orthogonal matrix $\widetilde{Q} = [\widetilde{Q}_1|\widetilde{Q}_2]$ such that

$$\left[\frac{V_{12}^{(q)}}{V_{22}^{(q)}}\right] \widetilde{Q} = [\; v_{p+1}, \ldots, v_{n+d} \;] \widetilde{Q} = \left[\begin{array}{c|c} \Omega & \widetilde{\Gamma} \\ \hline \widetilde{Y} & \widetilde{Z} \end{array}\right], \tag{3.18}$$

where $\widetilde{\Gamma} \in \mathbb{R}^{d \times d}$ is *nonsingular* and Ω is a matrix not necessarily equal to zero. Then define the correction matrix

$$\left[\, \widetilde{G} \mid \widetilde{E} \,\right] \equiv - \left[\, B \mid A \,\right] \left[\frac{\widetilde{\Gamma}}{\widetilde{Z}} \right] \left[\frac{\widetilde{\Gamma}}{\widetilde{Z}} \right]^T . \tag{3.19}$$

The corrected system $(A + \widetilde{E})X = B + \widetilde{G}$ is compatible and the matrix

$$\widetilde{X} \equiv -\widetilde{Z}\widetilde{\Gamma}^{-1} = -V_{22}^{(q)} \left(V_{12}^{(q)} \widetilde{Q}_2 \widetilde{Q}_2^T \right)^{\dagger} \tag{3.20}$$

solves this corrected system. The columns of $[\widetilde{\Gamma}^T | \widetilde{Z}^T]^T$ have to be in the null space of the corrected matrix $[B + \widetilde{G} | A + \widetilde{E}]$. As above, they do not necessarily represent a basis of this null space.

Now we show that $X^{(q)}$ does not necessarily represent a TLS solution, i.e., the Frobenius norm of the correction matrix (3.15) need not be minimal. This can be illustrated by a simple example. Let $q = n$ and $e < d$. Then in (3.13) we set $Q = [V_{22}^{(q)T} | V_{12}^{(q)T}]$. (Notice that $V_{11}^{(\Delta)}$ and $V_{21}^{(\Delta)}$ in the partitioning (2.6) vanish for $\Delta \equiv q = n$.) Therefore

$$\left[\frac{V_{12}^{(q)}}{V_{22}^{(q)}} \right] \left[\, V_{22}^{(q)T} \mid V_{12}^{(q)T} \,\right] = \left[\begin{array}{c|c} 0 & I_d \\ \hline I_n & 0 \end{array} \right], \qquad \text{i.e.,} \qquad \Gamma = I_d, \quad Z = 0,$$

which gives from (3.13) $[G|E] = -[B|0]$, and, analogously, $X^{(q)} = 0$, see (3.17). If we solve the same problem in the ordinary least squares sense, then the corresponding correction matrix is $[\bar{G}|\bar{E}] \equiv [(AA^{\dagger} - I)B|0]$ having in general smaller Frobenius norm than $[G|E] = -[B|0]$, given by (3.15). Therefore the constructed matrix $X^{(q)}$ given by (3.17) does not, in general, represent a TLS solution.

Summarizing, the classical TLS algorithm of Van Huffel computes for TLS problems of the 1st class the output (3.2), (3.10), or (3.17), which are formally analogous, but with different relationship to the TLS solution. While (3.2) and (in the particular case of a very special distribution of the singular values) (3.10) represent TLS solutions (having minimal Frobenius and 2-norm), the interpretation of (3.17) remains unclear. The partitioning of the set $\mathscr{F}$ of TLS problems of the 1st class according to the conditions valid in (3.2), (3.10), and (3.17) is unsatisfactory. In particular, apart from the simple case (3.2) and the very special case (3.10) we do not know whether a TLS solution exists.[1] We will therefore develop a different partitioning of the set $\mathscr{F}$ in Section 4. First we briefly discuss some properties of matrices $X^{(q)}$ and $\widetilde{X}$.

3.4. Note on the norms of matrices $X^{(q)}$ and $\widetilde{X}$. It is obvious that $X^{(q)}$ given by (3.17) is a special case of $\widetilde{X}$ given by (3.20). The following Lemma 3.5 gives simple formulas for the Frobenius norm and 2-norm of $\widetilde{X}$. Lemma 3.6 shows that $X^{(q)}$ has the minimal norms among all $\widetilde{X}$ of the form (3.20). The proofs are fully analogous to the proofs of [17, Theorems 3.6 and 3.9].

LEMMA 3.5. *Let $[\widetilde{\Gamma}^T | \widetilde{Z}^T]^T \in \mathbb{R}^{(n+d) \times d}$ have orthonormal columns and assume $\widetilde{\Gamma} \in \mathbb{R}^{d \times d}$ is nonsingular. Then the matrix $\widetilde{X} = -\widetilde{Z}\widetilde{\Gamma}^{-1}$ has the norms*

$$\|\widetilde{X}\|_F^2 = \|\widetilde{\Gamma}^{-1}\|_F^2 - d, \qquad \text{and} \qquad \|\widetilde{X}\|^2 = \frac{1 - \sigma_{\min}^2(\widetilde{\Gamma})}{\sigma_{\min}^2(\widetilde{\Gamma})}, \tag{3.21}$$

[1]The problems in the set $\mathscr{F}$ are in [17] called generic. Since a problem in this set may not have a TLS solution, we will not further use the generic-nongeneric terminology.

where $\sigma_{\min}(\widetilde{\Gamma})$ *is the minimal singular value of* $\widetilde{\Gamma}$.

LEMMA 3.6. *Consider* $X^{(q)} = -Z\Gamma^{-1} = -V_{22}^{(q)}V_{12}^{(q)\dagger}$ *given by (3.13)–(3.17) and* $\widetilde{X} = -\widetilde{Z}\widetilde{\Gamma}^{-1}$ *given by (3.18)–(3.20). Then*

$$\|\widetilde{X}\|_F \geq \|X^{(q)}\|_F, \qquad \text{and} \qquad \|\widetilde{X}\| \geq \|X^{(q)}\|. \tag{3.22}$$

Moreover, equality holds for the Frobenius norms if and only if $\widetilde{X} = X^{(q)}$.

These lemmas can be easily seen as follows. A matrix $\widetilde{X}$ of the form (3.20) is going to be minimal in the Frobenius or the 2-norm when $\|\widetilde{\Gamma}^{-1}\|_F$ is minimized or $\sigma_{\min}(\widetilde{\Gamma}) \equiv \sigma_d(\widetilde{\Gamma})$ is maximized, respectively. The minimization/maximization are with respect to the orthogonal matrix $\widetilde{Q}$ which is considered a free variable, with the constraint that $\widetilde{\Gamma}$ has to be nonsingular. The interlacing theorem for singular values applied to the matrices $[\Omega|\widetilde{\Gamma}] = V_{12}^{(q)}\widetilde{Q}$ and $\widetilde{\Gamma}$ gives

$$\sigma_j(\Gamma) = \sigma_j(V_{12}^{(q)}) = \sigma_j\left(\left[\begin{array}{c|c} \Omega & \widetilde{\Gamma} \end{array}\right]\right) \geq \sigma_j(\widetilde{\Gamma}), \qquad j = 1, \ldots, d,$$

with all the inequalities becoming equalities if and only if $\Omega = 0$. The minimum for the 2-norm is reached when the smallest singular values are equal, i.e., $\sigma_d(\Gamma) = \sigma_d(\widetilde{\Gamma})$. Note that there can be more than one matrix of the form (3.20) reaching the minimum of the 2-norm.

If the corrected matrix $(A+\widetilde{E})$ has linearly dependent columns, then the corrected system with the correction $[\widetilde{G}|\widetilde{E}]$ of the form (3.19) can have more than one solution. The following lemma shows that under some additional assumptions on the structure of $\widetilde{Q}$, the matrix $(A+\widetilde{E})$ is of full column rank, and therefore the matrix $\widetilde{X}$ of the form (3.20) is the unique solution of the corrected system. (Note that the correction (3.15) is a special case of the correction (3.19).)

LEMMA 3.7. *Consider a TLS problem of the 1st class. Let* $[\widetilde{G}|\widetilde{E}]$ *be the correction matrix given by (3.19) and let* $\widetilde{X}$ *be the matrix given by (3.20). If* $\widetilde{Q}$ *in (3.18) has the block diagonal form* $\widetilde{Q} = \mathrm{diag}(Q', I_{d-e})$, *where* $Q' \in \mathbb{R}^{(q+e)\times(q+e)}$ *is an orthogonal matrix, then* $(A+\widetilde{E})$ *is of full column rank and* $\widetilde{X}$ *represents the unique solution of the corrected system* $(A+\widetilde{E})\widetilde{X} = B+\widetilde{G}$.

Proof. Since $\widetilde{Q} = \mathrm{diag}(Q', I_{d-e})$ has the block diagonal structure,

$$\left[\begin{array}{c|c} B & A \end{array}\right] = U\Sigma V^T = \left(U\left[\begin{array}{c|c|c} I_p & 0 & 0 \\ \hline 0 & \widetilde{Q} & 0 \\ \hline 0 & 0 & I_{m-n-d} \end{array}\right]\right)\Sigma\left(V\left[\begin{array}{c|c} I_p & 0 \\ \hline 0 & \widetilde{Q} \end{array}\right]\right)^T \equiv \bar{U}\Sigma\bar{V}^T,$$

i.e. $\bar{U}\Sigma\bar{V}^T$ represents the SVD of $[B|A]$ with

$$\bar{U} = \left[\begin{array}{c} \bar{u}_1, \ldots, \bar{u}_m \end{array}\right], \qquad \bar{V} = \left[\begin{array}{c} \bar{v}_1, \ldots, \bar{v}_{n+d} \end{array}\right] = \left[\begin{array}{c||c|c} V_{11}^{(q)} & \Omega & \widetilde{\Gamma} \\ \hline V_{21}^{(q)} & \widetilde{Y} & \widetilde{Z} \end{array}\right].$$

Using this SVD, the corrected matrix can be written as

$$\left[\begin{array}{c|c} B+\widetilde{G} & A+\widetilde{E} \end{array}\right] = \left[\begin{array}{c} \bar{u}_1, \ldots, \bar{u}_n \end{array}\right]\mathrm{diag}(\sigma_1, \ldots, \sigma_n)\left[\begin{array}{c|c} V_{11}^{(q)} & \Omega \\ \hline V_{21}^{(q)} & \widetilde{Y} \end{array}\right]^T.$$

If $\sigma_n = 0$, then $[\widetilde{G}|\widetilde{E}] = 0$ and the original system is compatible, i.e. $\mathcal{R}(B) \subseteq \mathcal{R}(A)$; therefore assume $\sigma_n > 0$. From the CS decomposition of $\bar{V}$ it follows that since $\widetilde{\Gamma}$ is square nonsingular, the matrix $[V_{21}^{(q)}|\widetilde{Y}]$ is square nonsingular. Since $[\bar{u}_1, \ldots, \bar{u}_n]$ is of full column rank, the matrix

$$(A + \widetilde{E}) = \left[\ \bar{u}_1, \ldots, \bar{u}_n\ \right] \operatorname{diag}(\sigma_1, \ldots, \sigma_n) \left[\ V_{21}^{(q)} \mid \widetilde{Y}\ \right]^T$$

is of full column rank. The matrix $\widetilde{X}$ is then the *unique* solution of the corrected system $(A + \widetilde{E})\widetilde{X} = B + \widetilde{G}$. □

We will see in the next section that the form $\widetilde{Q} = \operatorname{diag}(Q', I_{d-e})$ appears in a natural way.

4. Partitioning of the set of problems of the 1st class. We will base our partitioning and the subsequent classification of TLS problems with multiple right-hand sides on the following theorem.

THEOREM 4.1. *Consider a TLS problem of the 1st class. Let (2.3) be the SVD of $[B|A]$ with the partitioning given by (2.6), $\Delta \equiv q \leq n$, where q is the "left multiplicity" of σ_{n+1} given by (2.5), $p \equiv n - q$. Consider an orthogonal matrix $\widetilde{Q}$ such that*

$$\left[\begin{array}{c} V_{12}^{(q)} \\ \hline V_{22}^{(q)} \end{array}\right] \widetilde{Q} = \left[\begin{array}{c|c} \Omega & \widetilde{\Gamma} \\ \hline \widetilde{Y} & \widetilde{Z} \end{array}\right], \qquad \widetilde{Q} = \left[\ \widetilde{Q}_1 \mid \widetilde{Q}_2\ \right], \tag{4.1}$$

where $\widetilde{Q}_1 \in \mathbb{R}^{(q+d)\times q}$, $\widetilde{Q}_2 \in \mathbb{R}^{(q+d)\times d}$, and define

$$\begin{aligned} \left[\ \widetilde{G} \mid \widetilde{E}\ \right] &\equiv -\left[\ B \mid A\ \right] \left[\begin{array}{c} \widetilde{\Gamma} \\ \hline \widetilde{Z} \end{array}\right] \left[\begin{array}{c} \widetilde{\Gamma} \\ \hline \widetilde{Z} \end{array}\right]^T \\ &= -\left[\ u_{p+1}, \ldots, u_{n+d}\ \right] \operatorname{diag}(\sigma_{p+1}, \ldots, \sigma_{n+d}) \widetilde{Q}_2 \widetilde{Q}_2^T \left[\ v_{p+1}, \ldots, v_{n+d}\ \right]^T. \end{aligned} \tag{4.2}$$

Then the following two assertions are equivalent:

(i) *There exists an orthonormal matrix $\Psi \in \mathbb{R}^{d\times d}$, such that $\widehat{Q} \equiv \widetilde{Q} \operatorname{diag}(I_q, \Psi)$ has the block diagonal structure*

$$\widehat{Q} = \left[\begin{array}{c|c} Q' & 0 \\ \hline 0 & I_{d-e} \end{array}\right] \in \mathbb{R}^{(q+d)\times(q+d)}, \qquad Q' \in \mathbb{R}^{(q+e)\times(q+e)}, \tag{4.3}$$

and using $\widehat{Q}$ in (4.1)–(4.2) instead of $\widetilde{Q}$ yields the same $[\widetilde{G}|\widetilde{E}]$.

(ii) *The matrix $[\widetilde{G}|\widetilde{E}]$ satisfies*

$$\left\| \left[\ \widetilde{G} \mid \widetilde{E}\ \right] \right\|_F = \left(\sum\nolimits_{j=n+1}^{n+d} \sigma_j^2 \right)^{1/2}. \tag{4.4}$$

Proof. First we prove the implication (i) $\Longrightarrow$ (ii). We partition $\widehat{Q} = [\widehat{Q}_1|\widehat{Q}_2]$, where $\widehat{Q}_1 \in \mathbb{R}^{(q+d)\times q}$, $\widehat{Q}_2 \in \mathbb{R}^{(q+d)\times d}$, and $Q' = [Q'_1|Q'_2]$, where $Q'_1 \in \mathbb{R}^{(q+e)\times q}$, $Q'_2 \in \mathbb{R}^{(q+e)\times e}$. Then

$$\widehat{Q}_2 \widehat{Q}_2^T = \left[\begin{array}{c|c} Q'_2 & 0 \\ \hline 0 & I_{d-e} \end{array}\right] \left[\begin{array}{c|c} Q'_2 & 0 \\ \hline 0 & I_{d-e} \end{array}\right]^T = \left[\begin{array}{c} Q'_2 \\ \hline 0 \end{array}\right] \left[\begin{array}{c} Q'_2 \\ \hline 0 \end{array}\right]^T + \left[\begin{array}{c} 0 \\ \hline I_{d-e} \end{array}\right] \left[\begin{array}{c} 0 \\ \hline I_{d-e} \end{array}\right]^T,$$

which gives, using (4.2) and (2.5)

$$\left\| \left[\begin{array}{c|c} \widetilde{G} & \widetilde{E} \end{array} \right] \right\|_F^2 = \|\mathrm{diag}(\sigma_{p+1}, \dots, \sigma_{n+d}) \widehat{Q}_2 \widehat{Q}_2^T \|_F^2$$
$$= \sigma_{n+1}^2 \|Q_2'(Q_2')^T\|_F^2 + \sum\nolimits_{j=n+e+1}^{n+d} \sigma_j^2 = \sigma_{n+1}^2 e + \sum\nolimits_{j=n+e+1}^{n+d} \sigma_j^2,$$

i.e. (4.4). The implication (i) $\Longrightarrow$ (ii) is proved.

Now we prove the implication (ii) $\Longrightarrow$ (i). Let $[\widetilde{G}|\widetilde{E}]$ be given by (4.1), (4.2) and assume that (4.4) holds. We prove that there exists $\widehat{Q}$ of the form (4.3) giving the same $[\widetilde{G}|\widetilde{E}]$. Define the splitting

$$\widetilde{Q} = \left[\begin{array}{c|c} \widetilde{Q}_1 & \widetilde{Q}_2 \end{array} \right] = \left[\begin{array}{c|c} \widetilde{Q}_{11} & \widetilde{Q}_{12} \\ \hline \widetilde{Q}_{21} & \widetilde{Q}_{22} \end{array} \right]$$

such that $\widetilde{Q}_{11} \in \mathbb{R}^{(q+e)\times q}$, $\widetilde{Q}_{21} \in \mathbb{R}^{(d-e)\times q}$, $\widetilde{Q}_{12} \in \mathbb{R}^{(q+e)\times d}$, $\widetilde{Q}_{22} \in \mathbb{R}^{(d-e)\times d}$. The matrix $[\widetilde{G}|\widetilde{E}]$ given by (4.2) satisfies

$$\left\| \left[\begin{array}{c|c} \widetilde{G} & \widetilde{E} \end{array} \right] \right\|_F^2 = \|\mathrm{diag}(\sigma_{p+1}, \dots, \sigma_{n+d}) \widetilde{Q}_2 \|_F^2$$
$$= \sigma_{n+1}^2 \|\widetilde{Q}_{12}\|_F^2 + \|D\widetilde{Q}_{22}\|_F^2,$$

where $D \equiv \mathrm{diag}(\sigma_{n+e+1}, \dots, \sigma_{n+d})$. Note that $\|\widetilde{Q}_{12}\|_F^2 = d - \|\widetilde{Q}_{22}\|_F^2$, since the matrix $\widetilde{Q}_2$ consists of d orthonormal columns. Thus

$$\left\| \left[\begin{array}{c|c} \widetilde{G} & \widetilde{E} \end{array} \right] \right\|_F^2 = \sigma_{n+1}^2 (d - \|\widetilde{Q}_{22}\|_F^2) + \|D\widetilde{Q}_{22}\|_F^2$$
$$= \sigma_{n+1}^2 d - \|(\sigma_{n+1}^2 I_{d-e} - D^2)^{1/2} \widetilde{Q}_{22}\|_F^2.$$

Using (4.4) this gives

$$\sigma_{n+1}^2 (d-e) - \sum\nolimits_{j=n+e+1}^{n+d} \sigma_j^2 = \|(\sigma_{n+1}^2 I_{d-e} - D^2)^{1/2} \widetilde{Q}_{22}\|_F^2.$$

Since $\sigma_{n+1} > \sigma_{n+e+\ell}$ for all $\ell = 1, \dots, d-e$, this implies that all rows of $\widetilde{Q}_{22}$ have norm equal to one. Consequently, since $\widetilde{Q}$ is an orthogonal matrix, $\widetilde{Q}_{21} = 0$, i.e.

$$\widetilde{Q} = \left[\begin{array}{c|c} \widetilde{Q}_1 & \widetilde{Q}_2 \end{array} \right] = \left[\begin{array}{c|c} \widetilde{Q}_{11} & \widetilde{Q}_{12} \\ \hline 0 & \widetilde{Q}_{22} \end{array} \right],$$

and the matrix $\widetilde{Q}_{22}$ has orthonormal rows. Consider the SVD $\widetilde{Q}_{22} = S[I_{d-e}|0]P^T = [S|0]P^T$, where $S \in \mathbb{R}^{(d-e)\times(d-e)}$, $P \in \mathbb{R}^{d\times d}$ are square orthogonal matrices. Define orthogonal matrices

$$\Psi \equiv P \left[\begin{array}{c|c} 0 & S^T \\ \hline I_e & 0 \end{array} \right] \in \mathbb{R}^{d\times d} \qquad \text{and} \qquad \widehat{Q} \equiv \widetilde{Q} \left[\begin{array}{c|c} I_q & 0 \\ \hline 0 & \Psi \end{array} \right] = \left[\begin{array}{c|c} \widetilde{Q}_{11} & \widetilde{Q}_{12}\Psi \\ \hline 0 & [0|I_{d-e}] \end{array} \right].$$

Because $\widehat{Q}$ is orthogonal, the last $d-e$ columns of $\widetilde{Q}_{12}\Psi$ (i.e. corresponding to the block I_{d-e}) are zero and

$$\widehat{Q} = \mathrm{diag}(Q', I_{d-e})$$

is in the form (4.3) with $Q' = [\widetilde{Q}_{11}|\widetilde{Q}_{12}\Psi I_{q+d}^{(e)}] \in \mathbb{R}^{(q+e)\times(q+e)}$, where $I_{q+d}^{(e)}$ represents the first e columns of I_{q+d}. Because $\widehat{Q}_2\widehat{Q}_2^T = (\widetilde{Q}_2\Psi)(\widetilde{Q}_2\Psi)^T = \widetilde{Q}_2\widetilde{Q}_2^T$, the matrix $\widehat{Q}$ yields the same correction (4.2) as $\widetilde{Q}$. ▯

The statement of this theorem says that *any* correction $[\widetilde{G}|\widetilde{E}]$ (reducing rank of $[B|A]$ to at most n) having the norm given by (4.4) can be obtained as in (4.1)–(4.2) with $\widetilde{Q}$ in the *block diagonal* form (4.3).

Now we describe three disjoint subsets of problems of the 1st class representing the core of the proposed classification. Define the partitioning of the matrix $V_{12}^{(q)}$ with respect to e, the "right multiplicity" of σ_{n+1}, given by (2.5)

$$V_{12}^{(q)} = \left[\begin{array}{c|c} \overbrace{\;W^{(q,e)}\;}^{q+e} & \overbrace{\;V_{12}^{(-e)}\;}^{d-e} \end{array}\right]\Big\}\, d\,, \tag{4.5}$$

where $W^{(q,e)} \in \mathbb{R}^{d\times(q+e)}$, $V_{12}^{(-e)} \in \mathbb{R}^{d\times(d-e)}$. Note that since $\mathrm{rank}(V_{12}^{(q)}) = d$, i.e. a problem is of the 1st class, $\mathrm{rank}(V_{12}^{(-e)}) \leq d - e$ implies that $\mathrm{rank}(W^{(q,e)}) \geq e$. On the other hand $\mathrm{rank}(W^{(q,e)}) = e$ implies that $\mathrm{rank}(V_{12}^{(-e)}) = d - e$.

Definition 4.2 (Partitioning of the set of problems of the 1st class). *Consider a TLS problem (1.1)–(1.3), $m \geq n + d$. Let (2.3) be the SVD of $[B|A]$ with the partitioning given by (2.6), $\Delta \equiv q$, and the partitioning of $V_{12}^{(q)}$ given by (4.5), where q and e are the integers related to the multiplicity of σ_{n+1}, given by (2.5). Let the problem (1.1)–(1.3) be of the 1st class (i.e., $\mathrm{rank}(V_{12}^{(q)}) = d$). The set of all problems for which*

- $\mathrm{rank}(W^{(q,e)}) = e$ *and* $\mathrm{rank}(V_{12}^{(-e)}) = d - e$ ($V_{12}^{(-e)}$ *has full column rank*),
- $\mathrm{rank}(W^{(q,e)}) > e$ *and* $\mathrm{rank}(V_{12}^{(-e)}) = d - e$ ($V_{12}^{(-e)}$ *has full column rank*),
- $\mathrm{rank}(W^{(q,e)}) > e$ *and* $\mathrm{rank}(V_{12}^{(-e)}) < d - e$ ($V_{12}^{(-e)}$ *is rank deficient*),

will be denoted by $\mathscr{F}_1$, $\mathscr{F}_2$, and $\mathscr{F}_3$, respectively. Clearly, $\mathscr{F}_1$, $\mathscr{F}_2$, and $\mathscr{F}_3$ are mutually disjoint and $\mathscr{F}_1 \cup \mathscr{F}_2 \cup \mathscr{F}_3 = \mathscr{F}$.

4.1. The set $\mathscr{F}_1$—problems of the 1st class having a TLS solution in the form $X^{(q)}$. Consider a TLS problem of the 1st class from the set $\mathscr{F}_1$, i.e. $\mathrm{rank}(W^{(q,e)}) = e$ in (4.5) which implies $V_{12}^{(-e)}$ is of full column rank, i.e. $\mathrm{rank}(V_{12}^{(-e)}) = d - e$. First we give a lemma which allows to relate the partitioning (4.5) to the construction of a solution in (3.13)–(3.17).

Lemma 4.3. *Let (2.3) be the SVD of $[B|A]$ with the partitioning (2.6), $m \geq n+d$, $\Delta \equiv q \leq n$. Consider the partitioning (4.5) of $V_{12}^{(q)}$. The following two assertions are equivalent:*

(i) *The matrix $W^{(q,e)}$ has rank equal to e.*
(ii) *There exists Q in the block diagonal form (4.3) satisfying (3.13).*

Proof. Let $W^{(q,e)} \in \mathbb{R}^{d\times(q+e)}$ have rank equal to e. Then $\mathrm{rank}(V_{12}^{(-e)}) = d - e$. There exists an orthogonal matrix $H \in \mathbb{R}^{(q+e)\times(q+e)}$ (e.g., a product of Householder transformation matrices) such that $W^{(q,e)}H = [0|M]$ where $M \in \mathbb{R}^{d\times e}$ is of full column rank. Putting $Q \equiv \mathrm{diag}(H, I_{d-e})$ yields $V_{12}^{(q)}Q = [0|\Gamma]$, where the square matrix $\Gamma \equiv [M|V_{12}^{(-e)}] \in \mathbb{R}^{d\times d}$ is nonsingular.

Conversely, let $Q = \mathrm{diag}(Q', I_{d-e})$ and satisfy (3.13). Denote $\Gamma = [\Gamma_1|\Gamma_2]$, where $\Gamma_1 \in \mathbb{R}^{d\times e}$, $\Gamma_2 \in \mathbb{R}^{d\times(d-e)}$. Obviously $[0|\Gamma_1] = W^{(q,e)}Q'$, $\Gamma_2 = V_{12}^{(-e)}I_{d-e} = V_{12}^{(-e)}$. Since Γ is nonsingular, $\mathrm{rank}(\Gamma_1) = e$. Q' is an orthogonal matrix and thus $\mathrm{rank}(W^{(q,e)}) = e$. □

The following theorem formulates results for the set $\mathscr{F}_1$.

THEOREM 4.4. *Let (2.3) be the SVD of $[B|A]$ with the partitioning (2.6), $m \geq n+d$, $\Delta \equiv q \leq n$ ($p \equiv n-q$). Let the TLS problem (1.1)–(1.3) be of the 1st class, i.e. $V_{12}^{(q)}$ is of full row rank equal to d. Let $\sigma_p > \sigma_{p+1} = \ldots = \sigma_{n+1} = \ldots = \sigma_{n+e}$, $1 \leq e \leq d$ (if $q = n$, then σ_p is not defined). Consider the partitioning of $V_{12}^{(q)}$ given by (4.5). If*

$$\mathrm{rank}(W^{(q,e)}) = e, \tag{4.6}$$

(the problem is from the set $\mathscr{F}_1$), then $X_{\mathrm{TLS}} \equiv X^{(q)} = -V_{22}^{(q)}V_{12}^{(q)\dagger}$ given by (3.17) represents the TLS solution having the minimality property (3.22). The corresponding correction $[G|E]$ given by (3.15) has the norm (4.4).

The proof follows immediately from Lemma 4.3, Lemma 3.6, and Lemma 3.7.

The problems of the 1st class discussed earlier in Sections 3.1 and 3.2 belong to the set $\mathscr{F}_1$. In the first case $q \equiv 0$ and $V_{12}^{(q)} \equiv V_{12}$ is square nonsingular. Thus independently on the value of e (4.5) yields $W^{(0,e)}$ with the (full column) rank equal to e and the matrix Q' from $Q = \mathrm{diag}(Q', I_{d-e})$ in the assertion (ii) of Lemma 4.3 can be always chosen equal to the identity matrix I_e, i.e. $Q = I_d$. In the second case $e \equiv d$. Thus $W^{(q,d)} \equiv V_{12}^{(q)}$ is of (full row) rank equal to d. Here the identity block I_{d-e} in the assertion (ii) of Lemma 4.3 disappears, i.e. $Q = Q'$.

4.2. The set $\mathscr{F}_2$—problems of the 1st class having a TLS solution but not in the form $X^{(q)}$. Consider a TLS problem of the 1st class from the set $\mathscr{F}_2$, i.e. $\mathrm{rank}(V_{12}^{(-e)}) = d - e$ and $\mathrm{rank}(W^{(q,e)}) > e$ in (4.5). Because $V_{12}^{(-e)}$ is of full column rank, there exists $\widetilde{Q} = \mathrm{diag}(Q', I_{d-e})$ having the block diagonal form (4.3) such that (4.1) holds,

$$V_{12}^{(q)}\widetilde{Q} = \left[\; W^{(q,e)}Q' \;\middle|\; V_{12}^{(-e)} \;\right] = \left[\; \Omega \;\middle\|\; \widetilde{\Gamma}_1 \;\middle|\; V_{12}^{(-e)} \;\right], \tag{4.7}$$

with $\widetilde{\Gamma} = [\widetilde{\Gamma}_1|V_{12}^{(-e)}]$ nonsingular. Consequently, the correction $[\widetilde{G}|\widetilde{E}]$ defined by (4.2) is minimal in the Frobenius norm, see Theorem 4.1, and the corresponding matrix $\widetilde{X} \equiv -\widetilde{Z}\widetilde{\Gamma}^{-1}$ given by (3.20) represents a TLS solution (which is, by Lemma 3.7, the unique solution of the corrected system with the given fixed correction $[\widetilde{G}|\widetilde{E}]$). Because $\mathrm{rank}(W^{(q,e)}) > e$ and Q' is orthogonal, the product $W^{(q,e)}Q' = [\Omega|\widetilde{\Gamma}_1]$ where $\mathrm{rank}(\widetilde{\Gamma}_1) = e$ ($\widetilde{\Gamma}$ is nonsingular) leads always to a nonzero Ω. On the other hand, the construction (3.15)–(3.17) always leads to $\Omega = 0$. Hence, the matrix $X^{(q)}$ given by (3.17) does not represent a TLS solution.

The following theorem completes the argument by showing that any problem from the set $\mathscr{F}_2$ has always a minimum norm TLS solution.

THEOREM 4.5. *Let (1.1)–(1.3) be the TLS problem of the 1st class belonging to the set $\mathscr{F}_2$. Then there exist TLS solutions given by (3.18)–(3.20) minimal in the 2-norm, and in the Frobenius norm, respectively.*

Proof. A TLS solution $\widetilde{X} = -\widetilde{Z}\widetilde{\Gamma}^{-1}$ is obtained from the formula

$$\left[\begin{array}{c} V_{12}^{(q)} \\ \hline V_{22}^{(q)} \end{array}\right] \widehat{Q} = \left[\begin{array}{c} V_{12}^{(q)} \\ \hline V_{22}^{(q)} \end{array}\right] \left[\begin{array}{c||c|c} Q_1' & Q_2' & 0 \\ \hline 0 & 0 & I_{d-e} \end{array}\right] = \left[\begin{array}{c|c} \Omega & \widetilde{\Gamma} \\ \hline \widetilde{Y} & \widetilde{Z} \end{array}\right],$$

where the block diagonal matrix $\widehat{Q}$ is the orthogonal matrix (4.3) from Theorem 4.1. The TLS solution is uniquely determined by the orthogonal matrix $Q' \equiv [Q_1'|Q_2'] \in \mathbb{R}^{(q+e)\times(q+e)}$.

In our construction, $Q' \in \mathbb{R}^{(q+e)\times(q+e)}$ is required to lead to a nonsingular $\widetilde{\Gamma}$. Since the matrix inversion is a continuous function of entries of a nonsingular matrix, and matrix multiplication is a continuous function of entries of both factors, the matrix $\widetilde{X} = -\widetilde{Z}\widetilde{\Gamma}^{-1}$ is a continuous matrix-valued function of Q'. Define two nonnegative functionals $\mathbf{N}_2(Q') : \mathbb{R}^{(q+e)\times(q+e)} \longrightarrow [0, +\infty]$ and $\mathbf{N}_F(Q') : \mathbb{R}^{(q+e)\times(q+e)} \longrightarrow [0, +\infty]$ on a set of all $(q+e)$-by-$(q+e)$ orthogonal matrices such that

$$\mathbf{N}_2(Q') \equiv \begin{cases} \|\widetilde{X}(Q')\|_2, & \text{if } Q' \text{ gives } \widetilde{\Gamma}(Q') \text{ nonsingular,} \\ +\infty, & \text{if } Q' \text{ gives } \widetilde{\Gamma}(Q') \text{ singular.} \end{cases}$$

The functional $\mathbf{N}_F(Q')$ is defined analogously. Note that both functionals are nonnegative and lower semi-continuous on the compact set of all $(q+e)$-by-$(q+e)$ orthogonal matrices, and thus both functionals have a minimum on this set. ◻

Theorem 4.5 does not address the uniqueness of the minimum norm solutions, and it also does not give any practical algorithm for computing them. Further note that the sets of solutions minimal in 2-norm and minimal in the Frobenius norm can be *different or even disjoint*. This fact can be illustrated with the following example. Consider the problem given by its SVD decomposition

$$[\ B \mid A\ ] \equiv U \left[\begin{array}{c|ccc} 3 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 1 \end{array}\right] \left(\frac{1}{4} \left[\begin{array}{c|ccc} -1 & -3 & \sqrt{3} & \sqrt{3} \\ 3 & -1 & \sqrt{3} & -\sqrt{3} \\ \hline \sqrt{3} & \sqrt{3} & 1 & 3 \\ \sqrt{3} & -\sqrt{3} & -3 & 1 \end{array}\right] \right)^T, \tag{4.8}$$

where $A \in \mathbb{R}^{4\times 2}$, $B \in \mathbb{R}^{4\times 2}$ (it is easy to verify that $A^T B \neq 0$). Here $q = 1$, $e = 1$,

$$W^{(q,e)} = \frac{1}{4}\begin{bmatrix} -3 & \sqrt{3} \\ -1 & \sqrt{3} \end{bmatrix}, \qquad V_{12}^{(-e)} = \frac{1}{4}\begin{bmatrix} \sqrt{3} \\ -\sqrt{3} \end{bmatrix},$$

have rank two and one, respectively. This problem is of the 1st class and belongs to the set $\mathscr{F}_2$. The TLS solution is determined by the orthogonal matrix

$$\widehat{Q} = \left[\begin{array}{c||c|c} Q_1' & Q_2' & 0 \\ \hline 0 & 0 & I_{d-e} \end{array}\right] = \left[\begin{array}{c||c|c} \cos(\phi) & -\sin(\phi) & 0 \\ \sin(\phi) & \cos(\phi) & 0 \\ \hline 0 & 0 & 1 \end{array}\right]$$

which depends only on one real variable ϕ. Figure 4.1 shows how the 2-norm and the Frobenius norm of the TLS solution depend on the value of ϕ. From the behavior of

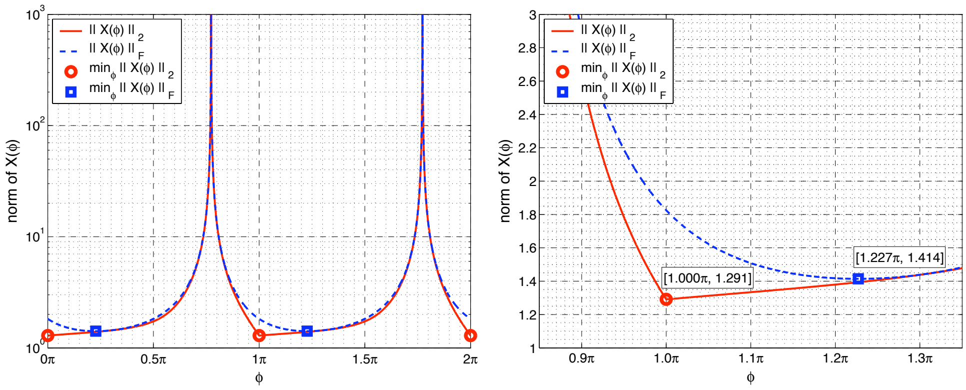


FIG. 4.1. *(Left plot) The* 2*-norm and the Frobenius norm of TLS solutions of the problem (4.8) belonging to the set* $\mathscr{F}_2$*. Solutions minimal in different norms are distinct. (Right plot) Detail of the solutions minimal in the 2-norm and in the Frobenius norm.*

the norms it is clear that the set of solutions minimal in 2-norm has no intersection with the set of solutions minimal in the Frobenius norm. If we use in the previous example (4.8) the matrix of the right singular vectors

$$V = \frac{1}{2}\left[\begin{array}{c|ccc} 0 & 1 & 0 & \sqrt{3} \\ -1 & 0 & \sqrt{3} & 0 \\ \hline \sqrt{3} & 0 & 1 & 0 \\ 0 & -\sqrt{3} & 0 & 1 \end{array}\right]$$

then there exists a solution which is minimal in both 2-norm and the Frobenius norm.

4.3. The set $\mathscr{F}_3$—problems of the 1st class which do not have a TLS solution. Consider a TLS problem of the 1st class from the set $\mathscr{F}_3$, i.e. the case with $\mathrm{rank}(V_{12}^{(-e)}) < d-e$. Since $V_{12}^{(-e)}$ in (4.5) is rank deficient, $\widetilde{Q} \in \mathbb{R}^{(q+d)\times(q+d)}$ in the block diagonal form (4.3) leads to (4.7) with $\widetilde{\Gamma} = [\,\widetilde{\Gamma}_1 | V_{12}^{(-e)}]$ containing linearly dependent column(s). Thus $\widetilde{\Gamma}$ in (4.1) is always singular. Consequently, in this case there does not exist $\widetilde{Q}$ in the block diagonal form yielding $\widetilde{\Gamma}$ nonsingular. Therefore, there is no correction $[\widetilde{G}|\widetilde{E}]$ having the norm (4.4) which makes the system (1.1) compatible, see Theorem 4.1.

Now we show that a TLS solution does not exist for the problems from the set $\mathscr{F}_3$. Using a general matrix $\widetilde{Q}$, see (3.18) we construct a correction (3.19) which makes the system compatible, and the norm of this correction is arbitrarily close to the lower bound (4.4). Denote $\rho \equiv (d-e) - \mathrm{rank}(V_{12}^{(-e)})$ the rank defect of $V_{12}^{(-e)}$. Analogously to Section 4.2, there exists an orthogonal matrix $Q' \in \mathbb{R}^{(q+e)\times(q+e)}$ such that

$$V_{12}^{(q)}\mathrm{diag}(Q', I_{d-e}) = \left[\; W^{(q,e)}Q' \;\middle|\; V_{12}^{(-e)} \;\right] = \left[\; \Omega \,\|\, \widetilde{\Gamma}_1 \;\middle|\; V_{12}^{(-e)} \;\right],$$

with $\mathrm{rank}([\widetilde{\Gamma}_1 | V_{12}^{(-e)}]) = d-\rho$, compare with (4.7). Let $\mathcal{J} = \{j_1, \ldots, j_\rho\}$ denote indices of any ρ columns of $V_{12}^{(-e)}$ such that the remaining columns of $V_{12}^{(-e)}$ (with indices $\{1, \ldots, d-e\} \setminus \mathcal{J}$) are linearly independent. Because $\mathrm{rank}(V_{12}^{(q)}) = d$, the matrix Ω has ρ linearly independent columns which are not in $\mathcal{R}([\widetilde{\Gamma}_1 | V_{12}^{(-e)}])$, let

$\mathcal{K} = \{k_1, \ldots, k_\rho\}$ denote their indices. Consider an angle θ, $0 < \theta < \pi$. A Givens rotation corresponding to θ applied subsequently on pairs of columns with indices j_ℓ and k_ℓ, for $\ell = 1, \ldots, \rho$, can be written as an orthogonal transformation

$$\left[\begin{array}{c||c|c} \Omega & \widetilde{\Gamma}_1 & V_{12}^{(-e)} \end{array}\right] \left[\begin{array}{c||c|c} C_{11} & 0 & S_{12} \\ \hline\hline 0 & I_e & 0 \\ \hline -S_{12}^T & 0 & C_{22} \end{array}\right] = \left[\begin{array}{c||c|c} \widehat{\Omega} & \widetilde{\Gamma}_1 & \widehat{V}_{12}^{(-e)} \end{array}\right],$$

where $C_{11} \in \mathbb{R}^{q \times q}$ and $C_{22} \in \mathbb{R}^{(d-e)\times(d-e)}$ are diagonal matrices having ρ diagonal entries (on the positions (k_ℓ, k_ℓ) and (j_ℓ, j_ℓ), $\ell = 1, \ldots, \rho$, respectively) equal to $\cos(\theta)$ (the other diagonal entries are equal to 1), and $S_{12} \in \mathbb{R}^{q\times(d-e)}$ has entries on positions (k_ℓ, j_ℓ), $\ell = 1, \ldots, \rho$, equal to $\sin(\theta)$ (the other entries are zero). Since $0 < \theta < \pi$, the matrix $\widetilde{\Gamma} = [\widetilde{\Gamma}_1 | \widehat{V}_{12}^{(-e)}]$ is nonsingular, and thus the corresponding correction makes the system compatible. The transformation matrix

$$\widetilde{Q} = \left[\begin{array}{c|c} Q'\mathrm{diag}(C_{11}, I_e) & Q'[\frac{S_{12}}{0}] \\ \hline [-S_{12}^T|0] & C_{22} \end{array}\right],$$

can be, with $\theta \longrightarrow 0$, arbitrarily close to the block diagonal form (4.3), and moreover the Frobenius norm of the corresponding correction

$$\left\| \left[\begin{array}{c|c} \widetilde{G} & \widetilde{E} \end{array}\right] \right\|_F = \left(\sum_{j=n+1}^{n+d} \sigma_j^2 + \sin^2(\theta) \sum_{j\in\mathcal{J}} (\sigma_{n+1}^2 - \sigma_{n+e+j}^2) \right)^{1/2}$$

can be arbitrarily close to the lower bound given by (4.4).

Consequently, there is *no minimal correction* that makes the system (1.1) compatible. The TLS problem (1.1)–(1.3) with rank deficient $V_{12}^{(-e)}$ does not have a solution.

4.4. Correction corresponding to the matrix $X^{(q)}$. In the previous three sections we have shown that a TLS solution (if exists) always has the correction matrix with the Frobenius norm (4.4). We can formulate the following Corollary.

COROLLARY 4.6. *Consider a TLS problem (1.1)–(1.3) of the 1st class. The construction (3.13)–(3.17) yields the TLS solution $X_{\mathrm{TLS}} \equiv X^{(q)}$ if and only if there exists an orthogonal matrix $\widehat{Q}$ in the block diagonal form (4.3) such that substituting $\widehat{Q}$ for Q in (3.13)–(3.15) gives the same correction $[G|E]$.*

Now we focus on the properties of the correction $[G|E]$ given by (3.15) in general. First we prove an auxiliary lemma.

LEMMA 4.7. *Let $[G|E]$ be the correction matrix given by (3.15). Denote $s \equiv$ $\mathrm{rank}([B|A])$. Then the ranks of the correction and corrected matrix satisfy*

$$\min\{s, d\} \geq \quad \mathrm{rank}\left(\left[\begin{array}{c|c} G & E \end{array}\right]\right) \quad \geq \max\{0, s-n\}, \tag{4.9}$$

$$\max\{0, s-d\} \leq \mathrm{rank}\left(\left[\begin{array}{c|c} B+G & A+E \end{array}\right]\right) \leq \min\{s, n\}. \tag{4.10}$$

Proof. The upper bound in (4.9) follows immediately from (3.15). The lower bound in (4.9) follows from the fact that the correction matrix makes the system compatible, i.e. the resulting rank of $[B+G|A+E]$ is at most n, which also proves the upper bound in (4.10). Since the rank of $[G|E]$ is at most d, the lower bounds in (4.10) follows trivially. $\square$

The result of the following theorem can also be found in [22, Equation (5.4)].

THEOREM 4.8. *Let $[G|E]$ be the correction matrix given by (3.15). Then its Frobenius norm satisfies*

$$\left(\sum_{j=p+1}^{p+d} \sigma_j^2\right)^{1/2} \geq \left\|\left[\ G \mid E\ \right]\right\|_F \geq \left(\sum_{j=n+1}^{n+d} \sigma_j^2\right)^{1/2}. \tag{4.11}$$

Proof. The lower bound in (4.11) is trivial. The matrix $[G|E]$ has from (4.9) the rank not greater than $\min\{s, d\}$ which immediately gives the upper bound. From the construction (3.15) a rank d matrix of the given form can not have Frobenius norm larger than (4.11). ∎

Since the Frobenius norm of the correction $[G|E]$ given by (3.15) can be larger than $(\sum_{j=n+1}^{n+d} \sigma_j^2)^{1/2}$, the correction need not be minimal and (3.17) need not represent (as described above) a TLS solution. Further note the inequalities in (4.11) become equalities if and only if

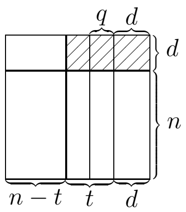
$$\sigma_{p+j} = \sigma_{n+j}, \qquad j = 1, \ldots, d,$$

(recall that $n = p + q$). This happens *either* if $q = 0$ (the case with the unique solution discussed in Section 3.1), *or* if $\sigma_{p+1} = \ldots = \sigma_{n+d}$ (the special case discussed in Section 3.2).

5. Problems of the 2nd class. In this section we briefly describe problems (1.1)–(1.3) of the 2nd class, i.e. the problems for which $V_{12}^{(q)}$ does not have full row rank, see Definition 2.2. Here the right singular vector subspace given by the last $(q + d)$ singular vectors $v_{p+1}, \ldots, v_{n+d}$ does not contain sufficient information for constructing a solution (3.20) and the problems of the 2nd class do not have a TLS solution (the argumentation is analogous as in Section 4.3).

The classical TLS algorithm, which gives an output also for problems of the 2nd class, is derived in [17] by a straightforward generalization of the single right-hand side concept. The right singular vector subspace $\mathcal{R}([V_{12}^{(q)T}|V_{22}^{(q)T}]^T)$ used for the construction (3.13)–(3.17) in previous cases is extended with additional right singular vectors until, for some t, a full row rank block $V_{12}^{(t)} \in \mathbb{R}^{d\times(t+d)}$ is found in the upper right corner of V (and $V_{12}^{(t-1)}$ is, at the same time, rank deficient),

$$V =$$



$$= \left[\begin{array}{c|c} V_{11}^{(t)} & V_{12}^{(t)} \\ \hline V_{21}^{(t)} & V_{22}^{(t)} \end{array}\right].$$

Then the matrix $X^{(t)} = -V_{22}^{(t)} V_{12}^{(t)\dagger}$ with the corresponding correction can be constructed analogously to (3.13)–(3.17), with q replaced by t. Obviously, this matrix might not be uniquely defined when σ_{n-t+1} is not simple, in particular, when $\sigma_{n-t} = \sigma_{n-t+1}$. In order to handle a possible multiplicity of σ_{n-t+1}, it is convenient to consider the following notation

$$\sigma_{n-\widetilde{q}} > \sigma_{n-\widetilde{q}+1} = \ldots = \sigma_{n-t} = \sigma_{n-t+1} \geq \sigma_{n-t+2},$$

where $\widetilde{q} \geq t$; put for simplicity $n - \widetilde{q} \equiv \widetilde{p}$. (If such $\sigma_{n-\widetilde{q}} \equiv \sigma_{\widetilde{p}}$ does not exist, then put $\widetilde{q} \equiv n$.) The condition that $V_{12}^{(\widetilde{q})}$ is of full row rank equal to d is readily satisfied, since $V_{12}^{(\widetilde{q})}$ extends $V_{12}^{(t)}$. Then $X^{(\widetilde{q})}$ and $[G|E]$ can be constructed as in (3.13)–(3.17) with q replaced by $\widetilde{q}$. Thus the matrix $X^{(\widetilde{q})} \equiv -V_{22}^{(\widetilde{q})} V_{12}^{(\widetilde{q})\dagger}$ represents a solution of the compatible corrected system $(A+E)X = B+G$. The Frobenius and the 2-norm of the matrix $X^{(\widetilde{q})}$ are given by Lemma 3.5. Similarly to the problems of the 1st class, the minimality property (3.22) of $X^{(\widetilde{q})}$ can be shown. Thus $X^{(\widetilde{q})}$ has minimal Frobenius and 2-norm over all matrices $\widetilde{X}$ that can be obtained from the construction analogous to (3.18)–(3.20) with q replaced by $\widetilde{q}$. The substitution of $\widetilde{q}$ for t ensures the uniqueness of the construction, and leads to the matrix with the smallest norm. On the other hand it inevitably increases the norm of the correction, with

$$\|[\ G \mid E\ ]\|_F > \left(\sum_{j=n+1}^{n+d} \sigma_j^2\right)^{1/2}.$$

The Frobenius norm of $[G|E]$ is strictly larger than the smallest possible correction reducing the rank of $[B|A]$ to n, and the matrix $X^{(\widetilde{q})}$ does not represent a TLS solution.[2]

6. Summary of the relationship to the classical TLS algorithm. The classical TLS algorithm gives for any data the output $X^{(\kappa)}$ which is equal (in exact

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Algorithm 1 (The classical TLS algorithm) A fully documented Fortran 77 implementation is given in [15, 16]. The code can be obtained through NETLIB.ORG, cf. `http://www.netlib.org/vanhuffel`.

Require: $A \in \mathbb{R}^{m\times n}$, $B \in \mathbb{R}^{m\times d}$ {here the SVD of $[B|A]$ in the form (2.3)–(2.6)}

$\Delta \leftarrow 0$

if $\operatorname{rank}(V_{12}^{(\Delta)}) = d$ **and** $\Delta = n$, **then goto** 6

if $\operatorname{rank}(V_{12}^{(\Delta)}) = d$ **and** $\sigma_{n-\Delta} > \sigma_{n-\Delta+1}$, **then goto** 6

$\Delta \leftarrow \Delta + 1$

goto 2

$\kappa \leftarrow \Delta$

$X^{(\kappa)} \leftarrow -V_{22}^{(\kappa)} V_{12}^{(\kappa)\dagger}$

return κ, $X^{(\kappa)}$

---

arithmetic) either to $X^{(q)}$ given by (3.2), or (3.10), or by (3.17), or to $X^{(\widetilde{q})}$ described in Section 5.

The output $X^{(\kappa)}$ is called generic (or TLS) solution in [17] for any problem of the 1st class, and it is called nongeneric solution in [17] for any problem of the 2nd class. As our new partitioning and the included classification reveals,

(i) if the problem is of the 1st class and $\operatorname{rank}(W^{(q,e)}) = e$, i.e., the problem belongs to the set $\mathscr{F}_1$, then $X^{(\kappa)} \equiv X_{\mathrm{TLS}}$ represents a TLS solution (it solves the TLS problem (1.1)–(1.3)), $\kappa \equiv q$,

(ii) if the problem is of the 1st class and $\operatorname{rank}(W^{(q,e)}) > e$, i.e., the problem belongs to the set $\mathscr{F}_2 \cup \mathscr{F}_3$, then $X^{(\kappa)}$ does not represent a TLS solution, which exists for the problems in the set $\mathscr{F}_2$ but does not exist for the problems in the set $\mathscr{F}_3$, $\kappa \equiv q$,

[2]The matrix $X^{(\widetilde{q})} = -V_{22}^{(\widetilde{q})} V_{12}^{(\widetilde{q})\dagger}$ is called *nongeneric solution* in [17, Definition 3.3, p. 78].

(iii) if the problem is of the 2nd class, i.e., the problem belong to the set $\mathscr{S}$, then $X^{(\kappa)}$ does not represent a TLS solution (a TLS solution does not exist), $\kappa \equiv \widetilde{q}$.

For $d = 1$ (single right-hand side case) the output $X^{(\kappa)}$ of Algorithm 1 represents the TLS solution of the core problem (3.5) transformed to the original coordinate system. The output $X^{(\kappa)}$ has two further important interpretations.

LEMMA 6.1 (The constrained total least squares (C-TLS)). *The matrix* $X^{(\kappa)} = -V_{22}^{(\kappa)} V_{12}^{(\kappa)\dagger}$ *given by Algorithm 1 represents the unique solution of the constrained minimization problem*

$$\min_{X,E,G} \| [\ G \mid E\ ] \|_F \qquad \textit{subject to} \qquad (A+E)X = B+G \tag{6.1}$$

$$\textit{and} \quad [\ G \mid E\ ] \left[\frac{0}{w} \right] = 0, \qquad \textit{for all} \qquad \left[\frac{0}{w} \right] \in \mathcal{R}\left(\left[\frac{V_{12}^{(\kappa)}}{V_{22}^{(\kappa)}} \right] \right), \tag{6.2}$$

with the correction $[G|E]$ *given by (3.15) (with* q *possibly replaced by* $\widetilde{q}$*).*

The additional constraint (6.2) can be equivalently rewritten as

$$[\ G \mid E\ ] \left[\frac{0}{Y} \right] = 0,$$

where Y is defined analogously to (3.13). Since $\sigma_{n-\kappa} > \sigma_{n-\kappa+1}$, the correction matrix in (6.1)–(6.2) is unique. Consequently, the constrained problem (6.1)–(6.2) has the unique solution $X_{\text{C-TLS}} \equiv X^{(\kappa)}$. Furthermore, since the matrix in (3.13) (with q possibly replaced by $\widetilde{q}$) has orthonormal columns, $X^{(\kappa)T} Y = -(\Gamma^{-1})^T Z^T Y = 0$, and the additional constraint implies that $X^{(\kappa)T} w = 0$ for all w from (6.2), see [17, Eq. 3.101, p. 79], [21, 22]. Note that the problem (6.1)–(6.2) for $\kappa \equiv \widetilde{q}$ is considered as a *definition* of the nongeneric solution in [17, Definition 3.3, p. 78 and Theorem 3.15, pp. 80–82].

LEMMA 6.2 (The truncated total least squares (T-TLS)). *The matrix* $X^{(\kappa)} = -V_{22}^{(\kappa)} V_{12}^{(\kappa)\dagger}$ *given by Algorithm 1 represents the unique minimum norm TLS solution of the modified TLS problem*

$$\min_{X,\widehat{E},\widehat{G}} \left\| \left[\ \widehat{G} \mid \widehat{E}\ \right] \right\|_F \qquad \textit{subject to} \qquad (\widehat{A}+\widehat{E})X = \widehat{B}+\widehat{G}, \tag{6.3}$$

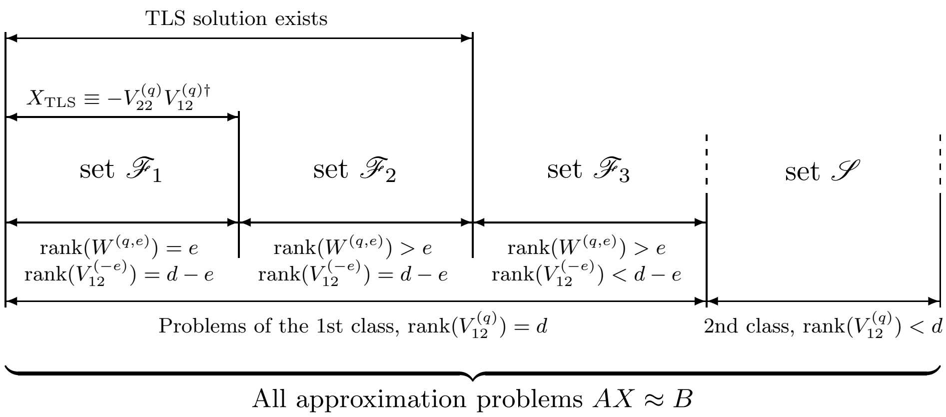
$$\textit{where} \quad \left[\ \widehat{B} \mid \widehat{A}\ \right] = \left(\sum\nolimits_{j=1}^{n-\kappa} u_j \sigma_j v_j^T \right) + \sigma_{n-\kappa+1} \left(\sum\nolimits_{j=n-\kappa+1}^{n+d} u_j v_j^T \right),$$

with the corresponding correction $[\widehat{G}|\widehat{E}]$*,* $\|[\widehat{G}|\widehat{E}]\|_F = \sigma_{n-\kappa+1}\sqrt{d}$*.*

The problem (6.3) is clearly a TLS problem of the 1st class (belonging to the set $\mathscr{F}_1$). Moreover it is a special case described in Section 3.2. This problem is called *truncated total least squares problem (T-TLS)* for the given A, B, with the solution $X_{\text{T-TLS}} \equiv X^{(\kappa)}$, see [17, note on p. 82]. It is worth to note that the T-TLS concept allows us to assume that the original problem $AX \approx B$ is a perturbation of the modified problem $\widehat{A}X \approx \widehat{B}$. From the T-TLS point of view, any TLS problem may be interpreted as a perturbed problem of the 1st class with the special singular values distribution (3.6). Since $X_{\text{T-TLS}} = X^{(\kappa)}$, Algorithm 1 can be used as a relatively simple and useful regularization technique, see, e.g., [21, 2, 3] (for $d = 1$) and also [17, Algorithm and comments in §3.6.1, pp. 87–90]. The distribution of the smallest singular values of $[B|A]$ plays no role in the algorithm output.

The *true* TLS solution (if it exists) does not have this regularization property. The TLS solution uses information about the smallest singular values of $[B|A]$.

7. Conclusions. We have presented a new classification of TLS problems with multiple right-hand sides. Each TLS problem falls into one of four distinct sets. The union of the first three sets $\mathscr{F}_j$, $j = 1, 2, 3$ contains problems of the 1st class. It is complemented by the set $\mathscr{S}$ of problems of the 2nd class, as illustrated by the following schema:



It has been shown that the special cases analyzed in [17] belong to the set $\mathscr{F}_1$. We have proved that *any* problem from $\mathscr{F}_1 \cup \mathscr{F}_2$ has a TLS solution, whereas problems from $\mathscr{F}_3 \cup \mathscr{S}$ do *not* have a TLS solution. Moreover, for any problem from $\mathscr{F}_1 \cup \mathscr{F}_2$ there exist a TLS solution minimal in the 2-norm and the solution minimal in the Frobenius norm, but for the problems from the set $\mathscr{F}_2$ the minimum norm solutions can be distinct.

The classical TLS algorithm (Algorithm 1) computes a TLS solution only for problems belonging to the set $\mathscr{F}_1$. We have not provided an efficient algorithm for computing a TLS solution for the problems from $\mathscr{F}_2$ (where it exists). It can possibly be obtained using a nonlinear optimization over a parameterization of the set of corresponding orthogonal matrices. However, this optimization is hardly practically applicable.

The TLS problems with $d = 1$ have been clarified through the concept of the *core reduction*. An extension of this concept to a TLS problems with $d > 1$ could help to understand the discrepancy between the true TLS solution and the solution given by the classical TLS algorithm. An approach based on such a reduction, outlined in [12], will be discussed elsewhere.

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