An Analysis of Rank-Deficient Scaled Total Least Squares Problem

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Abstract

In this paper, we study the scaled total least squares problems of rank-deficient linear systems. We present a solution for rank-deficient scaled total least squares and discuss the relation between scaled total least squares and least squares.


Keywords: Scaled total least squares, total least squares, least squares, rank-deficient.

1 Introduction

The least squares (LS) problem is to find $\mathbf{x}$ to minimize $\| \mathbf{b} - A\mathbf{x} \|_2$ for a given $A \in \mathbb{R}^{m \times n}$ ($m \geq n$) and a $\mathbf{b} \in \mathbb{R}^m$. Let the residual $\mathbf{r} = \mathbf{b} - A\mathbf{x}$, the least squares problem can be recast as

$$\min_{(\mathbf{b} - \mathbf{r}) \in \text{range}(A)} \| \mathbf{r} \|_2 \quad \text{for} \quad \mathbf{r} \in \mathbb{R}^n. \quad (1.1)$$

This formulation shows that the errors only occur on the vector $\mathbf{b}$. When $\mathbf{b} \in \text{range}(A)$, (1.1) is solved by $\mathbf{r}_{LS} = 0$. So, we assume $\mathbf{b} \not\in \text{range}(A)$ throughout this paper. The total least squares (TLS) problem allows errors to present in both $\mathbf{b}$ and $A$:

$$\min_{(\mathbf{b} - \mathbf{r}) \in \text{range}(A+E)} \| [E \mathbf{r}] \|_F \quad \text{for} \quad E \in \mathbb{R}^{m \times n} \quad \text{and} \quad \mathbf{r} \in \mathbb{R}^m. \quad (1.2)$$

When $A$ is of full column rank, $\text{rank}(A) = n$, the LS solution is unique and given by $\mathbf{x}_{LS} = (A^T A)^{-1} A^T \mathbf{b}$. When $A$ is rank-deficient, $\text{rank}(A) = k < n$, the LS solution
is not unique. The minimal 2-norm solution can be obtained by using the singular value decomposition (SVD) as follows. Suppose that

\[ A = \tilde{U} \begin{bmatrix} \hat{\Sigma} & 0 \\ 0 & 0 \end{bmatrix} \tilde{V}^T \]  

(1.3)

is the SVD of \( A \), where \( \tilde{U} \in \mathbb{R}^{m \times m} \) and \( \tilde{V} \in \mathbb{R}^{n \times n} \) are orthogonal and \( \hat{\Sigma} = \text{diag}(\tilde{\sigma}_1, ..., \tilde{\sigma}_k) \), \( \tilde{\sigma}_1 \geq \cdots \geq \tilde{\sigma}_k > 0 \). The minimal norm LS solution is given by

\[ x_{\text{LS}} = A^\dagger b \quad \text{where} \quad A^\dagger = \tilde{V} \begin{bmatrix} \hat{\Sigma}^{-1} & 0 \\ 0 & 0 \end{bmatrix} \tilde{U}^T \]

and the vector

\[ r_{\text{LS}} = b - Ax_{\text{LS}} = (I - AA^\dagger)b \]

solves (1.1).

For the TLS problem, we consider the SVD:

\[ [A \quad b] = \tilde{U} \hat{\Sigma} \tilde{V}^T, \]  

(1.4)

where \( \hat{\Sigma} = \text{diag}(\tilde{\sigma}_1, ..., \tilde{\sigma}_{n+1}) \), \( \tilde{\sigma}_1 \geq \cdots \geq \tilde{\sigma}_{n+1} \geq 0 \) and \( \tilde{U} \in \mathbb{R}^{m \times (n+1)} \) and \( \tilde{V} \in \mathbb{R}^{(n+1) \times (n+1)} \) have orthonormal columns, and partition

\[ \tilde{U} = \begin{bmatrix} \tilde{U}_1 & \tilde{u}_{n+1} \\ n & 1 \end{bmatrix} \quad \text{and} \quad \tilde{V} = \begin{bmatrix} \tilde{V}_{11} & \tilde{V}_{12} \\ \tilde{V}_{21} & \tilde{V}_{22} \end{bmatrix}, \]

\[ n \quad 1. \]

If \( \tilde{\sigma}_n > \tilde{\sigma}_{n+1} \), which implies that \( \tilde{\sigma}_n > 0 \) or \( A \) is of full column rank, then the matrix

\[ [E_{\text{TLS}} \quad r_{\text{TLS}}] = -\tilde{\sigma}_{n+1} \tilde{u}_{n+1} [\tilde{V}_{12}^T \tilde{v}_{22}] \]

solves (1.2) and

\[ x_{\text{TLS}} = -(A^T A - \tilde{\sigma}_{n+1}^2 I_n)^{-1} A^T b = -\tilde{v}_{12} / \tilde{v}_{22} \]

is the unique solution to \((A + E_{\text{TLS}}) x = b + r_{\text{TLS}} \) [2, Page 598].

If \( \tilde{\sigma}_n = \tilde{\sigma}_{n+1} \), then the solution to the TLS problem may still exist, although it may not be unique. Wei [10] considered the minimal norm TLS solution for a general case when

\[ \tilde{\sigma}_p > \tilde{\sigma}_{p+1} = \cdots = \tilde{\sigma}_q > \tilde{\sigma}_{q+1} \geq \cdots \geq \tilde{\sigma}_{n+1} \geq 0, \]

for some integers \( 1 \leq p \leq n \) and \( q > p \). For convenience, we restate the theorem for \( p = k \) and \( q = k + 1 \).

**Theorem 1.1** [10, Theorem 2.2] Partitioning \( \hat{\Sigma}, \tilde{U}, \) and \( \tilde{V} \) in (1.4):

\[ \hat{\Sigma} = \begin{bmatrix} \hat{\Sigma}_1 & 0 \\ 0 & \hat{\Sigma}_2 \end{bmatrix}, \quad \tilde{U} = \begin{bmatrix} \tilde{U}_1 & \tilde{U}_2 \end{bmatrix}, \quad (1.5) \]
and

\[
\hat{V} = \begin{bmatrix}
\hat{V}_{11} & \hat{V}_{12} \\
\hat{V}_{21} & \hat{V}_{22}
\end{bmatrix}^{n} k = n - k + 1
\]

(1.6)

if

\[
\hat{\sigma}_{k} > \hat{\sigma}_{k+1} > \hat{\sigma}_{k+2} \geq \cdots \geq \hat{\sigma}_{n+1} \geq 0
\]

then \( \hat{V}_{11} \) is of full column rank; \( \hat{V}_{22} \neq 0 \), and

\[
x_{TLS} = (\hat{V}_{11}^{T})^{\dagger} = \hat{V}_{11}^{T}/(1 - \hat{V}_{21}^{T} \hat{V}_{21})
\]

\[
= -\hat{V}_{12}^{T} = -\hat{V}_{12}^{T}/(1 - \hat{V}_{21}^{T} \hat{V}_{21})
\]

\[
= (A^{T}A - \hat{V}_{12}^{T} \hat{V}_{12})^{\dagger}(A^{T}b - \hat{V}_{12}^{T} \hat{V}_{22})
\]

(1.7)

is the minimal norm TLS solution. Moreover, let \( q = \hat{V}_{22}/\|\hat{V}_{22}\|_{2} \), then

\[
[E_{TLS} \ r_{TLS}] = \hat{U}^{T}_{2} \Sigma^{T}_{2} \Sigma^{T}_{2} \hat{V}_{12}^{T} \hat{V}_{22}
\]

solves (1.2) and

\[
\|[E_{TLS} \ r_{TLS}]\|_{F} = \hat{\sigma}_{k+1}.
\]

We refer the details of LS to [3] and TLS to [8]. The problems of LS and TLS can be unified by introducing a scaling parameter into the TLS problem. Rao [6] proposed

\[
\min_{(b-r) \in \text{range}(A+E)} \|[E \lambda r]\|_{F} \quad \text{for } E \in \mathbb{R}^{m \times n} \text{ and } r \in \mathbb{R}^{m},
\]

where \( \lambda > 0 \) is a given scalar. Paige and Strakos [5] suggested a slightly different but equivalent formulation:

\[
\min_{(\lambda b - r) \in \text{range}(A+E)} \|[E \lambda r]\|_{F}.
\]

If \([E_{TLS} \ r_{TLS}]\) solves the above problem (1.8), then the solution \(x_{TLS}\) for \(x\) in \((A + E_{TLS})\lambda x = \lambda b - r_{TLS}\) is called the scaled total least squares (STLS) solution. In this paper, we adopt the formulation (1.8) by Paige and Strakos.

Obviously, when \( \lambda = 1 \), the STLS (1.8) reduces to TLS. It is shown in [5] that \(x_{TLS}\) approaches \(x_{LS}\) as \( \lambda \rightarrow 0 \). In the STLS literatures [4, 5, 6], it is assumed that \(A\) is of full column rank. This paper presents the STLS solution when \(A\) is rank-deficient. The rest of the paper is organized as follows. In Section 2, we analyze the STLS when \(A\) is rank-deficient. Then in section 3, we relate STLS to LS.

2 Solving Rank-Deficient STLS

Following the STLS formulation (1.8), we denote

\[
C := [A \lambda b] = U\Sigma V^{T},
\]

(2.1)
where \( U \in \mathbb{R}^{m \times (n+1)} \) has orthonormal columns, \( V \in \mathbb{R}^{(n+1) \times (n+1)} \) orthogonal, and \( \Sigma = \text{diag}(\sigma_1, \ldots, \sigma_{n+1}) \), \( \sigma_1 \geq \cdots \geq \sigma_{k+1} > \sigma_{k+2} = \cdots = \sigma_{n+1} = 0 \). From Theorem 1.1, if \( \sigma_k > \sigma_{k+1} > 0 \), then, substituting \( \mathbf{b} \) in (1.2) with \( \lambda \mathbf{b} \), we can obtain the minimal norm STLS solution by applying the minimal norm TLS solution (1.7). Specifically, \( \lambda \mathbf{x}_{\text{STLS}} = \mathbf{x}_{\text{TLS}} \).

When does condition \( \sigma_k > \sigma_{k+1} \) hold? The following theorem gives a necessary and sufficient condition for \( \sigma_{k+1} = \bar{\sigma}_k \). The interlacing property says that \( \sigma_k \geq \bar{\sigma}_k \geq \sigma_{k+1} \). Thus, \( \bar{\sigma}_k \neq \sigma_{k+1} \) implies \( \sigma_k > \sigma_{k+1} \), which is what we need for applying Theorem 1.1 to STLS.

**Theorem 2.1** Suppose that \( A \) has the singular values
\[
\bar{\sigma}_1 \geq \cdots \geq \bar{\sigma}_j > \bar{\sigma}_{j+1} = \cdots = \bar{\sigma}_k > \bar{\sigma}_{k+1} = \cdots = \bar{\sigma}_n = 0
\]
for some \( j < k \) and \( \widehat{U} = [\mathbf{u}_1, \ldots, \mathbf{u}_m] \) is a column partition. Let
\[
\widehat{U}_k = [\mathbf{u}_{j+1}, \ldots, \mathbf{u}_k], \quad \rho := \|r_{z,s}\|_2, \quad \alpha_i := \mathbf{u}_i^T \mathbf{b}, \quad \text{for } i = 1, \ldots, k,
\]
and
\[
\psi(\sigma) = \lambda^2 \rho^2 - \sigma^2 - \lambda^2 \sigma^2 \sum_{i=1}^j \frac{\alpha_i^2}{\sigma_i^2 - \sigma^2}, \quad (2.2)
\]
then
\[
\sigma_{k+1} = \bar{\sigma}_k,
\]
if and only if
\[
\widehat{U}_k^T \mathbf{b} = 0, \quad \text{and} \quad \psi(\bar{\sigma}_k) \geq 0.
\]

**Proof.** We construct a matrix
\[
N = \widehat{U}^T C \begin{bmatrix} \widehat{V} & 0 \\ 0 & 1 \end{bmatrix}, \quad (2.3)
\]
which has the same singular values \( \bar{\sigma}_i \) as \( C \) in (2.1). Then, the \( n+1 \) eigenvalues of \( N^T N - \bar{\sigma}_k^2 I \) are
\[
\sigma_1^2 - \bar{\sigma}_k^2, \ldots, \sigma_k^2 - \bar{\sigma}_k^2, \quad \sigma_{k+1}^2 - \bar{\sigma}_k^2, \quad -\bar{\sigma}_k^2, \ldots, -\bar{\sigma}_k^2.
\]
From the interlacing property, the first \( k \) eigenvalues in the above list are nonnegative and there are exactly \( n-k \) negative eigenvalues if and only if \( \sigma_{k+1} = \bar{\sigma}_k \). In the following, we transform \( N^T N - \bar{\sigma}_k^2 I \) while keeping the number of the negative eigenvalues. First, to simplify \( N^T N - \bar{\sigma}_k^2 I \), recall that in the LS problem,
\[
r_{\text{LS}} = (I - AA^T) \mathbf{b} = \widehat{U} \begin{bmatrix} 0 & 0 \\ 0 & I_{m-k} \end{bmatrix} \widehat{U}^T \mathbf{b}.
\]
It then follows that
\[
\rho := \|r_{\text{LS}}\|_2 = \|[\mathbf{u}_{k+1}, \ldots, \mathbf{u}_m]^T \mathbf{b}\|_2.
\]
Defining
$$a = [\alpha_1, ..., \alpha_k]^T := [\bar{u}_1, ..., \bar{u}_k]^T b \quad \text{and} \quad \tilde{b} = [\bar{u}_{k+1}, ..., \bar{u}_m]^T b,$$
from (2.3) and (2.1), we have

$$N = \tilde{U}^T [A \lambda b] \begin{bmatrix} \hat{V} & 0 \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} \hat{\Sigma} & 0 & \lambda a \\ 0 & 0 & \lambda \tilde{b} \end{bmatrix} = \begin{bmatrix} I_k & 0 \\ 0 & H \end{bmatrix} \begin{bmatrix} \hat{\Sigma} & 0 & \lambda a \\ 0 & 0 & \lambda \tilde{b} \end{bmatrix},$$

where $H$ is a Householder matrix such that $H \tilde{b} = \rho e_1$. Thus

$$N^T N - \sigma_k^2 I = \begin{bmatrix} \hat{\Sigma} & 0 & \lambda a \\ 0 & 0 & \lambda \tilde{b} \end{bmatrix}^T \begin{bmatrix} \hat{\Sigma} & 0 & \lambda a \\ 0 & 0 & \lambda \tilde{b} \end{bmatrix} - \sigma_k^2 I$$

$$= \begin{bmatrix} \hat{\Sigma}^2 - \sigma_k^2 I_k & 0 & \lambda \hat{\Sigma} a \\ 0 & 0 & \lambda \hat{\Sigma} \tilde{b} \\ \lambda a^T \hat{\Sigma} & \lambda \hat{\Sigma} \tilde{b}^T & 0 \end{bmatrix}.$$ 

Partitioning
$$\hat{\Sigma} = \text{diag}(\hat{\Sigma}_1, \sigma_k I_{k-j}) \quad \text{where} \quad \hat{\Sigma}_1 = \text{diag}(\sigma_1, ..., \sigma_j),$$

and
$$a = \begin{bmatrix} a_1 \\ a_2 \end{bmatrix}$$

accordingly, we get

$$N^T N - \sigma_k^2 I = \begin{bmatrix} \hat{\Sigma}_1^2 - \sigma_k^2 I_j & 0 & 0 & \lambda \hat{\Sigma}_1 a_1 \\ 0 & 0 & 0 & \lambda \hat{\Sigma} a_2 \\ 0 & 0 & -\sigma_k^2 I_{n-k} & 0 \\ \lambda a_1^T \hat{\Sigma}_1 & \lambda \hat{\Sigma}_1 a_2^T & 0 & \lambda^2 (\rho^2 + a^T a) - \sigma_k^2 \end{bmatrix}.$$ 

Now, it can be verified that the Schur complement of $\hat{\Sigma}_1^2 - \sigma_k^2 I_j$ is

$$M := \begin{bmatrix} 0 & 0 & \lambda \hat{\Sigma}_1 a_2 \\ 0 & -\sigma_k^2 I_{n-k} & 0 \\ \lambda \hat{\Sigma}_1 a_2^T & 0 & \psi(\sigma_k) + \lambda^2 a_2^T a_2 \end{bmatrix}, \quad (2.4)$$

since

$$\lambda^2 (\rho^2 + a^T a) - \sigma_k^2 - \lambda^2 a_1^T \hat{\Sigma}_1 (\hat{\Sigma}_1^2 - \sigma_k^2 I_j)^{-1} \hat{\Sigma}_1 a_1$$

$$= \lambda^2 a_2^T a_2 + \lambda^2 \rho^2 - \sigma_k^2 + \lambda^2 a_1^T a_1 - \lambda^2 a_1^T \hat{\Sigma}_1^2 (\hat{\Sigma}_1^2 - \sigma_k^2 I_j)^{-1} a_1$$

$$= \lambda^2 a_2^T a_2 + \psi(\sigma_k).$$
Since $\bar{\Sigma}^2 - \tilde{\sigma}_k^2 I_j$ is positive definite, from Sylvester law of inertia [2, Page 403], the number of the negative eigenvalues of $N^T N - \tilde{\sigma}_k^2 I$ equals the number of the negative eigenvalues of $M$, which, from (2.4), has exactly $n - k$ negative eigenvalues if and only if

$$M_1 := \begin{bmatrix} 0 & \lambda \tilde{\sigma}_k a_2 \\ \lambda \tilde{\sigma}_k a_2^T & \psi(\tilde{\sigma}_k) + \lambda^2 a_2^T a_2 \end{bmatrix}$$

is positive semi-definite. It follows from Lemma 3.1 in [5] that $M_1$ is positive semi-definite if and only if

$$0 = a_2 = \tilde{U}_k^T b \quad \text{and} \quad \psi(\tilde{\sigma}_k) \geq 0.$$

This completes the proof. \[\square\]

The condition $\tilde{\sigma}_k > \sigma_{k+1}$ for the existence of the minimal norm STLS solution requires the singular values of both $A$ and $C$. This theorem provides the alternative conditions $\tilde{U}_k^T b \neq 0$ and $\psi(\tilde{\sigma}_k) < 0$ which require only the SVD of $A$. From this theorem, if $\tilde{U}_k^T b \neq 0$ or $\psi(\tilde{\sigma}_k) < 0$, then we can apply Theorem 1.1 to STLS. For example, if $\Sigma, U,$ and $V$ in (2.1) are partitioned as in (1.5) and (1.6), then, from (1.7), the minimal norm STLS solution $x_{\text{stls}}$ can be given by

$$\lambda x_{\text{stls}} = (V_{11}^T) v_{21} = -V_{12} (v_{22}^T)^T = (A^T A - V_{12} \Sigma_2 \Sigma_2 v_{22}^T) (\lambda A^T b - V_{12} \Sigma_2 v_{22}).$$

Moreover, let $q = v_{22} / \|v_{22}\|_2$, then

$$[E_{\text{stls}} \ r_{\text{stls}}] = U_2 \Sigma_2 q q^T [V_{12}^T \ v_{22}]$$

solves (1.8) and

$$\| [E_{\text{stls}} \ r_{\text{stls}}] \|_F = \sigma_{k+1}.$$

Finally, we conclude this section by presenting two properties of $\sigma_{k+1}$.

**Corollary 2.2** If $\tilde{U}_k^T b \neq 0$ or $\psi(\tilde{\sigma}_k) < 0$, then $\sigma_{k+1}$ is the smallest positive solution for $\sigma$ in $\psi(\sigma) = 0$ defined in (2.2).

**Proof.** On the one hand, the matrix $N$ defined in (2.3) has the singular values $\sigma_1 \geq \cdots \geq \sigma_{k+1}$. Thus, $\sigma_{k+1}$ is the smallest positive solution for $\sigma$ in the equation $\det(N^T N - \sigma^2 I) = 0$.

On the other hand, we consider

$$N^T N - \sigma^2 I = \begin{bmatrix} \tilde{\Sigma}^2 - \sigma^2 I_k & 0 & \lambda \tilde{\Sigma} a \\ 0 & -\sigma^2 I_{n-k} & 0 \\ \lambda a^T \tilde{\Sigma} & 0 & \lambda^2 (\rho^2 + a^T a) - \sigma^2 \end{bmatrix}.$$

Similar to (2.4), the Schur complement of $\tilde{\Sigma}^2 - \sigma^2 I_k$ is

$$\begin{bmatrix} -\sigma^2 I_{n-k} & 0 \\ 0 & \psi(\sigma) \end{bmatrix},$$

and...
since
\[
\lambda^2(\rho^2 + a^T a) - \sigma^2 - \lambda^2 a^T \Sigma (\Sigma^2 - \sigma^2 I_k)^{-1} \Sigma a
\]
\[
= \lambda^2 \rho^2 - \sigma^2 + \lambda^2 a^T \Sigma (\Sigma^2 - \sigma^2 I_k)^{-1} a
\]
\[
= \psi(\sigma).
\]
Thus, we have
\[
\det(N^T N - \sigma^2 I) = (-1)^{n-k} \sigma^{2(n-k)} \psi(\sigma) \det(\Sigma^2 - \sigma^2 I_k).
\]

From Theorem 2.1, when \( \tilde{U}_k^T b \neq 0 \) or \( \psi(\tilde{\sigma}_k) < 0 \), we have \( \tilde{\sigma}_k > \sigma_{k+1} \). Consequently, \( \Sigma^2 - \sigma_{k+1}^2 I_k \) is positive definite. Therefore, \( \sigma_{k+1} \) is the smallest positive solution for \( \sigma \) in the equation \( \psi(\sigma) = 0 \), because it is the smallest positive solution for \( \sigma \) in the equation \( \det(N^T N - \sigma^2 I) = 0 \). \( \square \)

**Corollary 2.3** Under the condition that \( \tilde{U}_k^T b \neq 0 \) or \( \psi(\tilde{\sigma}_k) < 0 \), \( \sigma_{k+1} \) is a monotonically increasing function of \( \lambda \).

**Proof.** From Corollary 2.2, under the given condition, \( \psi(\sigma_{k+1}) = 0 \). Differentiating
\[
0 = \psi(\sigma_{k+1})/(\lambda^2 \sigma_{k+1}^2),
\]
with respect to \( \lambda \), we get
\[
0 = -\frac{2 \rho^2 \sigma'_{k+1}}{\sigma_{k+1}^3} + \frac{2}{\lambda^3} - \sum_{i=1}^j \frac{2 \alpha_i^2 \sigma_{k+1} \sigma'_{k+1}}{\sigma_{k+1}^2 - \sigma_{k+1}^2}
\]
\[
= \frac{2}{\lambda^3} - 2 \sigma'_{k+1} \left( \frac{\rho^2}{\sigma_{k+1}^3} + \sigma_{k+1} \sum_{i=1}^j \frac{\alpha_i^2}{\sigma_{k+1}^2 - \sigma_{k+1}^2} \right),
\]
which implies \( \sigma'_{k+1} > 0 \), since \( \lambda > 0 \) and the value of the expression in the square bracket is positive. \( \square \)

## 3 Relating STLS to LS

The relation between STLS and TLS is obvious. The TLS problem is a special case of STLS when \( \lambda = 1 \). In this section, we discuss the relation between STLS and LS. It is shown in [5] that \( x_{\text{stls}} \) approaches to \( x_{\text{ls}} \) as \( \lambda \) tends to zero when \( A \) is of full column rank and \( \tilde{U}_k^T b \neq 0 \). In this section, we extend their result to the case when \( A \) is rank-deficient.

**Theorem 3.1** If \( \tilde{U}_k b \neq 0 \) or \( \psi(\tilde{\sigma}_k) < 0 \), then
\[
\lim_{\lambda \to 0} x_{\text{stls}} = x_{\text{ls}} \quad \text{and} \quad \lim_{\lambda \to 0} \frac{\sigma_{k+1}}{\lambda} = \rho.
\]
Proof. We first show that
\[
\lim_{\lambda \to 0} \frac{\sigma_{k+1}^2}{\lambda} = 0.
\]
Indeed, from Corollary 2.2, we have
\[
\sigma_{k+1}^2 = \lambda^2 \left( \rho^2 - \sigma_{k+1}^2 \sum_{i=1}^{j} \frac{\alpha_i^2}{\sigma_i^2 - \sigma_{k+1}^2} \right). \tag{3.1}
\]
It follows that \( \lim_{\lambda \to 0} (\sigma_{k+1}^2/\lambda) = 0 \), which implies \( \lim_{\lambda \to 0} \sigma_{k+1}^2 = 0 \). Then, noting that \( \Sigma_2 = \text{diag}(\sigma_{k+1},0,...,0) \) and \( (A^T A)^T = A^t \), from (2.5), we have
\[
\lim_{\lambda \to 0} x_{\text{STLS}} = \lim_{\lambda \to 0} (A^T A - V_{12} \Sigma_2^2 V_{12}^T)^t (A^T b - \lambda^{-1} V_{12} \Sigma_2 \Sigma_2^2 V_{22}) = (A^T A)^t A^t b = x_{\text{LS}} .
\]
Also, from (3.1), we get
\[
\lim_{\lambda \to 0} \frac{\sigma_{k+1}}{\lambda} = \lim_{\lambda \to 0} \sqrt{\rho^2 - \sigma_{k+1}^2 \sum_{i=1}^{j} \frac{\alpha_i^2}{\sigma_i^2 - \sigma_{k+1}^2}} = \rho . \tag*{\qed}
\]
In the following, we derive bounds for \( \|x_{\text{STLS}} - x_{\text{LS}}\|_2 \) and the residual norm \( \|b - Ax_{\text{STLS}}\|_2 \).

Theorem 3.2 \( \text{If } \hat{U}_k b \neq 0 \text{ or } \psi(\hat{\sigma}_k) < 0, \text{ then} \)
\[
\|x_{\text{STLS}} - x_{\text{LS}}\|_2 \leq \frac{\sigma_{k+1}}{\sigma_k} \|V_{12}^T x_{\text{STLS}} - \lambda^{-1} \Sigma_2 \Sigma_2^2 V_{22}\|_2 + \beta \|x_{\text{STLS}}\|_2 \leq \left( \frac{\sigma_{k+1}}{\sigma_k} + \beta \right) \frac{1}{\lambda \|\Sigma_2 \Sigma_2^2 V_{22}\|_2} ,
\]
where
\[
\beta = \min \left( 1, \frac{\sigma_{k+1}}{\sigma_k} \right). \tag{3.2}
\]
Also, the residual norm
\[
\|b - Ax_{\text{STLS}}\|_2 \leq \rho + \frac{\sigma_{k+1}}{\lambda \sigma_k \|\Sigma_2 \Sigma_2^2 V_{22}\|_2} . \tag{3.3}
\]
Proof. First, we show some equalities used in our derivation. Partitioning \( \Sigma, U, \) and \( V \) in the SVD (2.1) of \( C \) as \( \hat{\Sigma}, \hat{U}, \) and \( \hat{V} \) in (1.5) and (1.6), we can verify
\[
A^T A = V_{11} \Sigma_1^2 V_{11}^T + V_{12} \Sigma_2^2 V_{12}^T, \quad \lambda A^T b = V_{11} \Sigma_1^2 v_{21} + V_{12} \Sigma_2^2 v_{22} . \tag{3.3}
\]
and 
$$V_{12}^T V_{12} + v_{22} v_{22}^T = I.$$  
(3.4)

From the generalized inverse theory [9], we have

$$(A^T A)^+ A^T = A^+,$$  
(3.5) $$\quad (I - A^+ A) A^T = 0$$

and 
$$x^+ = x^T/(x^T x), \quad x \neq 0.$$  
(3.6)

Then, using the first equation in (3.5), $x_{LS} = A^T b = (A^T A)^+ A^T b$ and the second equation in (3.3), we get

$$x_{STLS} - x_{LS} = (I - A^+ A)x_{STLS} + (A^T A)^+ V_{12}^2 V_{12}^T x_{STLS} + (A^T A)^+ (A^T A) x_{STLS} - (A^T A)^+ A^T b = (A^T A)^+ [A^T A - V_{12}^2 V_{12}^T] x_{STLS} - \lambda^{-1} V_{11}^2 V_{11}^T v_{21} - \lambda^{-1} (A^T A)^+ V_{12}^2 V_{12}^T v_{22} + (I - A^+ A)x_{STLS} + (A^T A)^+ V_{12}^2 V_{12}^T x_{STLS}.$$  

From the first equation in (3.3) and $\lambda x_{STLS} = (V_{11}^T)^+ v_{21}$ in (2.5), the expression in the square bracket in the above equation:

$$(A^T A - V_{12}^2 V_{12}^T) x_{STLS} - \lambda^{-1} V_{11}^2 V_{11}^T v_{21} = \lambda^{-1} V_{11}^2 V_{11}^T v_{21} - \lambda^{-1} V_{11}^2 V_{11}^T v_{21} = 0,$$

since $V_{11}^T (V_{11}^T)^+ = I$, because, applying Theorem 1.1, $V_{11}$ is of full column rank. Thus

$$x_{STLS} - x_{LS} = (I - A^+ A)x_{STLS} + (A^T A)^+ V_{12}^2 V_{12}^T x_{STLS} - \lambda^{-1} V_{11}^2 V_{11}^T v_{22}.$$  
(3.7)

In the following, we show that the first term on the right side of (3.7) satisfies $\| (I - A^+ A) x_{STLS} \|_2 \leq \beta \| x_{STLS} \|_2$, where $\beta$ is defined in (3.2).

On the one hand, $\| (I - A^+ A) x_{STLS} \|_2 \leq \| x_{STLS} \|_2$ since $I - A^+ A$ is an orthogonal projection. On the other hand, (2.5) and the symmetry of $A^T A - V_{12}^2 V_{12}^T$ imply that

$$x_{STLS} = (A^T A - V_{12}^2 V_{12}^T)^+ (A^T A - V_{12}^2 V_{12}^T)^+ x_{STLS} = (A^T A - V_{12}^2 V_{12}^T)^+ (A^T A - V_{12}^2 V_{12}^T)^+ x_{STLS}.$$  

Hence, from the second equation in (3.5),

$$\| (I - A^+ A) x_{STLS} \|_2$$

$$= \| (I - A^+ A)(A^T A - V_{12}^2 V_{12}^T)(A^T A - V_{12}^2 V_{12}^T)^+ x_{STLS} \|_2$$

$$= \| (I - A^+ A)V_{12}^2 V_{12}^T (A^T A - V_{12}^2 V_{12}^T)^+ x_{STLS} \|_2$$

$$\leq \| V_{12}^2 V_{12}^T \|_2 \| (A^T A - V_{12}^2 V_{12}^T)^+ \|_2 \| x_{STLS} \|_2$$

$$\leq \sigma_{k+1}^2 \| (A^T A - V_{12}^2 V_{12}^T)^+ \|_2 \| x_{STLS} \|_2.$$  
(3.8)
Now, we claim that
\[
\| (A^T A - V_{12} \Sigma_2^2 V_{12}^T)^\dagger \|_2 \leq \frac{1}{\sigma_k^2 - \sigma_{k+1}^2},
\]
then we have \( \|(J - A^\dagger A) x_{\text{STLS}}\|_2 \leq \beta \|x_{\text{STLS}}\|_2 \). Indeed, from the first equation in (3.3), \( A^T A - V_{12} \Sigma_2^2 V_{12}^T \) is of rank \( k \), so
\[
\| (A^T A - V_{12} \Sigma_2^2 V_{12}^T)^\dagger \|_2 = \frac{1}{\sigma_k (A^T A - V_{12} \Sigma_2^2 V_{12}^T)}.
\]
From Mirsky theorem [7, Page 204], we have
\[
\sigma_k(A^T A - V_{12} \Sigma_2^2 V_{12}^T) - \sigma_k(A^T A) \geq -\|V_{12} \Sigma_2^2 V_{12}^T\|_2 \geq -\sigma_{k+1}^2
\]
and consequently
\[
\| (A^T A - V_{12} \Sigma_2^2 V_{12}^T)^\dagger \|_2 = \frac{1}{\sigma_k (A^T A - V_{12} \Sigma_2^2 V_{12}^T)} \leq \frac{1}{\sigma_k^2 - \sigma_{k+1}^2}.
\]
For the second term on the right side of (3.7), from \( \lambda x_{\text{STLS}} = -V_{12}(v_{22}^T)^\dagger \) in (2.5), (3.4), and (3.6), we have
\[
V_{12}^T x_{\text{STLS}} - \lambda^{-1} v_{22}
= -\lambda^{-1} (V_{12}^T V_{12}(v_{22}^T)^\dagger + v_{22})
= -\lambda^{-1} (V_{12}^T V_{12} + v_{22} v_{22}^T) v_{22}/(v_{22}^T v_{22})
= -\lambda^{-1} (v_{22}^T)^\dagger,
\]
which implies
\[
\| (A^T A)^\dagger V_{12} \Sigma_2^2 (V_{12}^T x_{\text{STLS}} - \lambda^{-1} v_{22}) \|_2 
\leq \frac{\sigma_{k+1}^2}{\sigma_k^2} \| V_{12}^T x_{\text{STLS}} - \lambda^{-1} v_{22} \|_2 
= \frac{\sigma_{k+1}^2}{\lambda \sigma_k^2} \| v_{22} \|_2 = \frac{\sigma_{k+1}^2}{\lambda \sigma_k^2} \| v_{22} \|_2.
\]
(3.8)
Putting things together, we get
\[
\| x_{\text{STLS}} - x_{\text{LS}} \|_2 \leq \frac{\sigma_{k+1}^2}{\lambda \sigma_k^2} \| v_{22} \|_2 + \beta \| x_{\text{STLS}} \|_2 \leq \left( \frac{\sigma_{k+1}^2}{\lambda \sigma_k^2} + \beta \right) \frac{1}{\lambda \| v_{22} \|_2} \lambda,
\]
since \( \| \lambda x_{\text{STLS}} \|_2 = \| V_{12}(v_{22}^T)^\dagger \|_2 \leq \| v_{22}^\dagger \|_2 = \| v_{22} \|_2^{-1} \).

Finally, using (3.7) and (3.8), we get the residual norm
\[
\| b - Ax_{\text{STLS}} \|_2 
\leq \| b - A x_{\text{LS}} \|_2 + \| A(A^T A)^\dagger V_{12} \Sigma_2^2 (V_{12}^T x_{\text{STLS}} - \lambda^{-1} v_{22}) \|_2 
\leq \rho + \frac{\sigma_{k+1}^2}{\lambda \sigma_k} \| v_{22} \|_2 = \rho + \frac{\sigma_{k+1}^2}{\lambda \sigma_k} \| v_{22} \|_2.
\]
\( \square \)
Conclusion

In this paper, we showed the conditions for the existence of the minimal norm solution for rank-deficient STLS. Our conditions involve only the SVD of the coefficient matrix A. Also, we gave explicit forms of the minimal norm solution for rank-deficient STLS. In Section 3 we showed the difference norm $\|x_{\text{STLS}} - x_{\text{LS}}\|$ between an STLS solution and its corresponding LS solution and the STLS residual norm $\|b - Ax_{\text{STLS}}\|$.

References


