A contribution to the condition number of the total least squares problem

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Abstract

This paper concerns cheaply computable formulas and bounds for the condition number of the TLS problem. For a TLS problem with data \( A, b \), two formulas are derived that are simpler and more compact than the known results in the literature. One is derived by exploiting the properties of Kronecker products of matrices. The other is obtained by making use of the singular value decomposition (SVD) of \([A b]\), which allows us to compute the condition number cheaply and accurately. We present lower and upper bounds for the condition number that involve the singular values of \([A b]\) and the last entries of the right singular vectors of \([A b]\). We prove that they are always sharp and can estimate the condition number accurately by no more than four times. Furthermore, we establish a few other lower and upper bounds that involve only a few singular values of \( A \) and \([A b]\). We discuss how tight the bounds are. These bounds are particularly useful for large scale TLS problems since for them any formulas and bounds for the condition number involving all the singular values of \( A \) and/or \([A b]\) are too costly to be computed. Numerical experiments illustrate that our bounds are sharper than a known approximate condition number in the literature.

Keywords: total least squares, condition number, singular value decomposition.

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1 Introduction

For given \( A \in \mathbb{R}^{m \times n} (m > n) \), \( b \in \mathbb{R}^m \), the TLS problem can be formulated as (see, e.g., [5, 12])

\[
\min \| [E \ r] \|_F, \quad \text{subject to} \quad b - r \in \mathcal{R}(A + E),
\]

where \( \| \cdot \|_F \) denotes the Frobenius norm of a matrix and \( \mathcal{R}(\cdot) \) denotes the range space. Suppose that \([E_{TLS} \ r_{TLS}]\) solves the above problem. Then \( x = x_{TLS} \) that satisfies the equation \((A + E_{TLS})x = b - r_{TLS}\) is called the TLS solution of (1).

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The condition number measures the worst-case sensitivity of a solution of a problem to small perturbations in the input data. Combined with backward errors, it provides an approximate local linear upper bound on the computed solution. Since the 1980’s, algebraic perturbation analysis for the TLS problem has been studied extensively; see [3, 5, 9, 13, 16] and the references therein. In recent years, asymptotic perturbation analysis and TLS condition numbers have been studied; see, e.g., [1] [8, 18].

In the present paper, we continue our work in [8] that studied the condition number of the TLS problem. We will derive a number of results. Firstly, we establish two formulas that are simpler and more suitable for computational purpose than the known results in the literature. One is derived by exploiting the properties of Kronecker products of matrices. It improves the formulas given in [8, 15], is independent of Kronecker products of matrices and makes its computation convenient. The other is obtained by making use of the SVD of \([A b]\), which can be used to compute the condition number more cheaply and accurately than that in [1]. Secondly, we present lower and upper bounds for the condition number that involve the singular values of \([A b]\) and the last entries of the right singular vectors of \([A b]\). We prove that these bounds are always sharp and can estimate the condition number accurately by no more than four times. Finally, we focus on cheaply computable bounds of the TLS condition number. We establish lower and upper bounds that involve only a few singular values of \(A\) and \([A b]\). We discuss how tight the bounds are. These bounds are particularly useful for large scale TLS problems since for them any formulas and bounds for the condition number involving all the singular values of \(A\) and/or \([A b]\) are too costly to be computed. So we can compute these bounds by calculating only a few singular values of \(A\) and/or \([A b]\) using some iterative solvers for large SVDs. In [2], an approximate TLS condition number is presented and is applied to evaluate conditioning of the TLS problem there. In this paper, we present numerical experiments to demonstrate a possibly great improvement of one of our upper bounds over the approximate condition number in [2].

The paper is organized as follows. In Section 2, we give some preliminaries necessary. In Section 3, we present computable formulas of the TLS condition number. The straightforward bounds on the TLS condition number are considered in Section 4. In Section 5, we present numerical experiments to show the tightness of bounds for the TLS condition number. We end the paper with some concluding remarks in Section 6.

Throughout the paper, for given positive integers \(m, n\), \(\mathbb{R}^n\) denotes the space of \(n\)-dimensional real column vectors, \(\mathbb{R}^{m \times n}\) denotes the space of all \(m \times n\) real matrices. \(\| \cdot \|\) and \(\| \cdot \|_F\) denote 2-norm and Frobenius norm of their arguments, respectively. Given a matrix \(A\), \(A(1 : i, 1 : i)\) is a Matlab notation that denotes the \(i\)th leading principal submatrix of \(A\), and \(\sigma_i(A)\) denotes the \(i\)th largest singular value of \(A\). For a vector \(a\), \(a(i)\) denotes the \(i\)th component of \(a\), and \(\text{diag}(a)\) is a diagonal matrix whose diagonals are given as components of \(a\). \(I_n\) denotes the \(n \times n\) identity matrix, \(O_{mn}\) denotes the \(m \times n\) zero matrix, whereas \(O\) denotes a zero matrix whose order is clear from the context. For matrices \(A = [a_1, \ldots, a_n] = [A_{ij}] \in \mathbb{R}^{m \times n}\) and \(B\), \(A \otimes B = [A_{ij}B]\) is the Kronecker product of \(A\) and \(B\), the linear operator \(\text{vec} : \mathbb{R}^{m \times n} \rightarrow \mathbb{R}^{mn}\) is defined by \(\text{vec}(A) = [a_1^T, \ldots, a_n^T]^T\) for \(A \in \mathbb{R}^{m \times n}\).
2 Preliminaries

Throughout the paper, we let $\hat{U}^T A \hat{V} = \text{diag}(\hat{\sigma}_1, \ldots, \hat{\sigma}_n)$ be the thin SVD of $A \in \mathbb{R}^{m \times n}$, where $\hat{\sigma}_1 \geq \cdots \geq \hat{\sigma}_n$, $\hat{U} \in \mathbb{R}^{m \times n}$, $\hat{U}^T \hat{U} = I_n$, $\hat{V} \in \mathbb{R}^{n \times n}$, $\hat{V}^T \hat{V} = I_n$. Let $U^T [A b] V = \text{diag}(\sigma_1, \ldots, \sigma_{n+1})$ be the thin SVD of $[A b] \in \mathbb{R}^{m \times (n+1)}$, where $\sigma_1 \geq \cdots \geq \sigma_{n+1}$, $U = [u_1, \ldots, u_{n+1}] \in \mathbb{R}^{m \times (n+1)}$, $U^T U = I_{n+1}$, $V = [v_1, \ldots, v_{n+1}] \in \mathbb{R}^{(n+1) \times (n+1)}$, $V^T V = I_{n+1}$.

The following result presents an existence and uniqueness condition for the TLS solution [5].

Theorem 1 If

$$\sigma_{n+1} < \hat{\sigma}_n,$$

then the TLS problem (1) has a unique solution $x_{\text{TLS}}$. Moreover,

$$x_{\text{TLS}} = (A^T A - \sigma_{n+1}^2 I)^{-1} A^T b = \left[ \frac{v_{n+1}(1)}{v_{n+1}(n+1)}, \ldots, \frac{v_{n+1}(n)}{v_{n+1}(n+1)} \right]^T.$$  (4)

In the paper, it is always assumed that condition (2) holds. We note that, for a given TLS problem (1), if $\sigma_{n+1} = 0$, then $b \in \mathbb{R}(A)$. In this case, the system of equations $Ax = b$ is compatible, and we can take $[E r] = O$. As in [5, 13], in the sequel, we do not consider this trivial case and assume that

$$0 < \sigma_{n+1} < \hat{\sigma}_n.$$  (5)

We will use the following properties of the TLS problem, which are in [5]:

$$\sigma_{n+1}^2 = \frac{\|r\|^2}{1 + \|x\|^2}.$$  (6)

and

$$A^T r = \frac{\|r\|^2}{1 + \|x\|^2} x = \sigma_{n+1}^2 x,$$  (7)

where $x = x_{\text{TLS}}$, $r = Ax - b$. By (4), it holds that

$$v_{n+1} = \frac{1}{\sqrt{1 + \|x\|^2}} \begin{bmatrix} x \\ -1 \end{bmatrix}$$  (8)

up to a sign $\pm 1$.

The following basic properties of the Kronecker products of matrices are needed later and can be found in [6]:

$$(A \otimes C)(B \otimes D) = (AB) \otimes (CD),$$

$$(A \otimes B)^T = A^T \otimes B^T,$$

where $A, B, C, D$ are matrices with appropriate sizes.
3 Computable formulas for the TLS condition number

Throughout the paper, we follow the definition of condition number in [4, 13]. Let \( g : \mathbb{R}^p \rightarrow \mathbb{R}^q \) be a continuous map in normed linear spaces defined on an open set \( D_g \subset \mathbb{R}^p \). For a given \( a \in D_g \), \( a \neq 0 \), with \( g(a) \neq 0 \), if \( g \) is differentiable at \( a \), then the relative condition number of \( g \) at \( a \) is

\[
\kappa^r_g(a) = \frac{\|g'(a)\|\|a\|}{\|g(a)\|} \tag{9}
\]

and the absolute condition number of \( g \) is

\[
\kappa_g(a) = \|g'(a)\|, \tag{10}
\]

where \( g'(a) \) denotes the derivative of \( g \) at \( a \).

Given the TLS problem (1), let \( \tilde{A} = A + \Delta A \), \( \tilde{b} = b + \Delta b \), where \( \Delta A \) and \( \Delta b \) denote the perturbations in \( A \) and \( b \), respectively. Consider the perturbed TLS problem

\[
\min \| [E \ r] \|_F \text{ subject to } \tilde{b} - \tilde{r} \in \mathcal{R}(\tilde{A} + E). \tag{11}
\]

In [8], we have established the following result.

**Theorem 2** Suppose the TLS problem (1) satisfies (5). Denote by \( x_{TLS} \) the TLS solution, and define \( r = Ax - b \), \( G(x) = [x^T - 1] \otimes I_m \). If \( \|[\Delta A \ \Delta b]\|_F \) is small enough, then the perturbed problem (11) has a unique TLS solution \( \tilde{x}_{TLS} \). Moreover,

\[
\tilde{x}_{TLS} = x_{TLS} + K \begin{bmatrix} \text{vec}(\Delta A) \\ \Delta b \end{bmatrix} + O(\|[\Delta A \ \Delta b]\|_F^2), \tag{12}
\]

where

\[
K = (A^TA - \sigma^2_{n+1}I_n)^{-1} \left( 2A^T \frac{r}{\|r\|} \frac{r^T}{\|r\|}G(x) - A^TG(x) - [I_n \otimes r^T O] \right). \tag{13}
\]

Denote \( a = \text{vec}(A) \). Based on Theorem 2 in a small neighborhood of \( [a^T, b^T]^T \in \mathbb{R}^{m(n+1)} \), we can define the function

\[
g : \mathbb{R}^{m(n+1)} \rightarrow \mathbb{R}^n
\]

\[
\begin{bmatrix} \tilde{a} \\ \tilde{b} \end{bmatrix} \mapsto \tilde{x} = (\tilde{A}^T \tilde{A} - \tilde{\sigma}^2_{n+1}I_n)^{-1} \tilde{A}^T \tilde{b},
\]

where \( \tilde{a} = a + \text{vec}(\Delta A) = \text{vec}(\tilde{A}) \), \( \tilde{b} = b + \Delta b \), and \( \tilde{x} \) is the solution to the perturbed TLS problem (11). In particular, \( g([a^T, b^T]^T) = x \). Thus, we have the following theorem.

**Theorem 3** Let \( \kappa_g(A, b) \) and \( \kappa^r_g(A, b) \) be the absolute and relative condition numbers of the TLS problem, respectively. Then

\[
\kappa_g(A, b) = \|K\|, \quad \kappa^r_g(A, b) = \frac{\|K\|[A \ b]_F}{\|x\|}, \tag{14}
\]

where \( K \) is defined as in (13).
Proof. By the definition of \( g \) and \([12]\), we see that \( g \) is differentiable at \([a^T, b^T]^T\) and 
\[ g'( [a^T, b^T]^T ) = K. \]
Then the assertion follows from \([9] \) and \([10] \) \( \square \).

The dependence of Kronecker product of matrices for \( K \) makes the computation of \( \kappa_g(A, b) \) via \([12] \) too costly. The same are the formulas given in \([8, 18] \). For a computational purpose, we will present a new formula of \( \kappa_g(A, b) \) that has a simpler and clearer form. To this end, we need a lemma.

Lemma 1 Let
\[
C = A^T A + \sigma^2_{n+1} I_n - \frac{2 \sigma^2_{n+1} x x^T}{\|x\|^2 + 1}. 
\]
Then \( C \) is positive definite.

Proof. Noticing that
\[
C = A^T A - \sigma^2_{n+1} I_n + 2 \sigma^2_{n+1} \left( I_n - \frac{x x^T}{1 + \|x\|^2} \right), \tag{15}
\]
and that \( A^T A - \sigma^2_{n+1} I_n \) and \( I_n - \frac{x x^T}{1 + \|x\|^2} \) are both positive definite, we complete the proof of the lemma. \( \square \)

Theorem 4 Let \( A^T A + \sigma^2_{n+1} I_n - \frac{2 \sigma^2_{n+1} x x^T}{\|x\|^2 + 1} = LL^T \) be the Cholesky factorization. Then
\[
\kappa_g(A, b) = \sqrt{\|x\|^2 + 1 \left\| (A^T A - \sigma^2_{n+1} I_n)^{-1} L \right\|}. \tag{16}
\]

Proof. Consider expression \([13] \) of \( K \). By the properties of Kronecker product of matrices, we get
\[
G(x)G^T(x) = ([x^T - 1] \otimes I_m) \left( \begin{bmatrix} x \\ -1 \end{bmatrix} \otimes I_m \right) = (\|x\|^2 + 1) I_m,
\]
\[
[I_n \otimes r^T O]G^T(x) = [I_n \otimes r^T O] \left[ \begin{bmatrix} x \otimes I_m \\ -I_m \end{bmatrix} \right] = (I_n \otimes r^T)(x \otimes I_m) = x r^T
\]
and
\[
[I_n \otimes r^T O] \left[ \begin{bmatrix} I_n \otimes r \\ O \end{bmatrix} \right] = (I_n \otimes r^T)(I_n \otimes r) = \|r\|^2 I_n. 
\]

Thus, we have
\[
\left( 2A^T \frac{r}{\|r\|} \frac{r^T}{\|r\|} G(x) - A^T G(x) - [I_n \otimes r^T O] \right) 
\cdot \left( 2G^T(x) \frac{r}{\|r\|} \frac{r^T}{\|r\|} A - G^T(x) A - [I_n \otimes r \frac{r^T}{\|r\|} O] \right) 
= (\|x\|^2 + 1) A^T A + \|r\|^2 I_n - x r^T A - A^T r x^T 
= (\|x\|^2 + 1) A^T A + \|r\|^2 I_n - 2 \sigma^2_{n+1} x x^T. 
\]
The last equality used $A^T r x^T = \sigma_{n+1}^2 x x^T$, which follows from (17). Denote $P = A^T A - \sigma_{n+1}^2 I_n$. We get

$$KK^T = P^{-1} ((\|x\|^2 + 1)A^T A + \|r\|^2 I_n - 2\sigma_{n+1}^2 x x^T) P^{-1}$$

$$= (\|x\|^2 + 1)P^{-1} \left(A^T A + \sigma_{n+1}^2 I_n - \frac{2\sigma_{n+1}^2 x x^T}{\|x\|^2 + 1}\right) P^{-1}. \quad (18)$$

In the last equality we used (6). From Theorem 3, we have

$$\kappa_g(A, b) = (\|x\|^2 + 1)^{\frac{1}{2}} \left\|P^{-1} \left(A^T A + \sigma_{n+1}^2 I_n - \frac{2\sigma_{n+1}^2 x x^T}{\|x\|^2 + 1}\right) P^{-1}\right\|^{\frac{1}{2}}. \quad (19)$$

Based on Lemma [1] we complete the proof.

Compared with the formula of $\kappa_g(A, b)$ in Theorem 3, the formula in Theorem 4 does not involve the Kronecker product of matrices and makes its computation convenient. However, if $\sigma_n$ and $\sigma_{n+1}$ are close, then $A^T A - \sigma_{n+1}^2 I_n$ becomes ill conditioned. Therefore, it may be hard to use (10) to calculate $\kappa_g(A, b)$ accurately. Next we derive a new formula that can be used to compute the condition number accurately.

**Theorem 5** Let $U^T [A \ b] V = \text{diag}(\sigma_1, \ldots, \sigma_{n+1})$ be the SVD of $[A \ b]$ with $V = [v_1, \ldots, v_{n+1}]$. Denote $V_{11} = V(1 : n, 1 : n)$. Then

$$\kappa_g(A, b) = \sqrt{\|x\|^2 + 1} \left\|V_{11}^{-1} S\right\|,$$

where $S = \text{diag}([s_1, \ldots, s_n])$, $s_i = \sqrt{\frac{\sigma_i^2 + \sigma_{n+1}^2}{\sigma_i^2 - \sigma_{n+1}^2}}$, $i = 1, \ldots, n$.

**Proof.** Denote $P = A^T A - \sigma_{n+1}^2 I_n$. From (18), we have

$$\frac{1}{\|x\|^2 + 1} K K^T = P^{-1} + 2\sigma_{n+1}^2 P^{-1} \left(I_n - \frac{x x^T}{1 + \|x\|^2}\right) P^{-1}. \quad (20)$$

Note that

$$[A \ b]^T [A \ b] - \sigma_{n+1}^2 I_{n+1} = \sum_{i=1}^{n+1} \sigma_i^2 v_i v_i^T - \sigma_{n+1}^2 \sum_{i=1}^{n+1} v_i v_i^T$$

$$= \sum_{i=1}^{n} (\sigma_i^2 - \sigma_{n+1}^2) v_i v_i^T.$$

We get

$$P = A^T A - \sigma_{n+1}^2 I_n = [I_n \ 0] \sum_{i=1}^{n} (\sigma_i^2 - \sigma_{n+1}^2) v_i v_i^T \begin{bmatrix} I_n \\ 0 \end{bmatrix}$$

$$= [I_n \ 0] [v_1, \ldots, v_n] \begin{bmatrix} \sigma_1^2 - \sigma_{n+1}^2 \\ \vdots \\ \sigma_n^2 - \sigma_{n+1}^2 \end{bmatrix} \begin{bmatrix} v_1^T \\ \vdots \\ v_n^T \end{bmatrix} [I_n \ 0]$$

$$= V_{11} \begin{bmatrix} \sigma_1^2 - \sigma_{n+1}^2 \\ \vdots \\ \sigma_n^2 - \sigma_{n+1}^2 \end{bmatrix} V_{11}^T := V_{11} A V_{11}^T. \quad (21)$$
Similarly, by (8), since \( v_{n+1} = \frac{1}{\sqrt{1 + \|x\|^2}} \begin{bmatrix} x \\ -1 \end{bmatrix} \), we have
\[
I_{n+1} - \frac{1}{1 + \|x\|^2} \begin{bmatrix} xx^T & -x \\ -x & 1 \end{bmatrix} = I_{n+1} - v_{n+1}v_{n+1}^T = [v_1, \ldots, v_n] \begin{bmatrix} v_1^T \\ \vdots \\ v_n^T \end{bmatrix}
\]
and
\[
I_n - \frac{xx^T}{1 + \|x\|^2} = V_{11}V_{11}^T.
\] (22)

By (22), we see that \( V_{11} \) is invertible. Combining (21) and (22), we have
\[
P^{-1} + 2\sigma^2_{n+1}P^{-1} \left( I_n - \frac{xx^T}{1 + \|x\|^2} \right) P^{-1} = V_{11}^T\Lambda^{-1}V_{11}^{-1} + 2\sigma^2_{n+1} \left( V_{11}^T\Lambda^{-1}V_{11}^{-1} \right) V_{11}V_{11}^T \left( V_{11}^T\Lambda^{-1}V_{11}^{-1} \right)
\]
\[
= V_{11}^T\Lambda^{-1}V_{11}^{-1} + 2\sigma^2_{n+1} V_{11}^T\Lambda^{-2}V_{11}^{-1}
\]
\[
= V_{11}^T \left( \Lambda^{-1} + 2\sigma^2_{n+1}\Lambda^{-2} \right) V_{11}^{-1} = \left( V_{11}^T S \right) \left( V_{11}^T S \right)^T. \] (23)

Then by (20) and Theorem 3 we get the desired equality. \( \square \)

By Theorem 5, we can calculate \( \kappa_g(A, b) \) by solving a linear system with the coefficient matrix \( V_{11}^T \). Next we show what the condition number of \( V_{11}^T \) is exactly.

**Theorem 6** For \( V_{11} \), we have
\[
\sigma_1(V_{11}) = 1, \ldots, \sigma_{n-1}(V_{11}) = 1, \sigma_n(V_{11}) = \frac{1}{\sqrt{1 + \|x\|^2}} \] (25)
and
\[
\kappa(V_{11}^T) = \frac{\sigma_1(V_{11})}{\sigma_n(V_{11})} = \sqrt{1 + \|x\|^2}. \] (26)

**Proof.** By the definition of \( V_{11} \) and the interlacing property [17, p.103] for eigenvalues of symmetric matrices, we get
\[
\sigma_1(V_{11}) = 1, \ldots, \sigma_{n-1}(V_{11}) = 1.
\]
Noticing that
\[
V_{11}V_{11}^T x = \left( I_n - \frac{1}{1 + \|x\|^2} xx^T \right) x = x - \frac{\|x\|^2}{1 + \|x\|^2} x = \frac{1}{1 + \|x\|^2} x,
\]
we know that \( \frac{1}{1 + \|x\|^2} \) is an eigenvalue of \( V_{11}V_{11}^T \), that is, \( \sigma_n(V_{11}) = \frac{1}{\sqrt{1 + \|x\|^2}} \). Thus, we have proved (25) and (26). \( \square \)

A different SVD-based closed formula for \( \kappa_g(A, b) \) appears in [1]. It is shown in [1] that
\[
\kappa_g(A, b) = \sqrt{\|x\|^2 + 1} \left\| \hat{D} \left[ \hat{V}^T O_{n,1} \right] V \left[ D \ 0_{n,1} \right]^T \right\|, \] (27)

\[7\]
where
\[ \hat{D} = \text{diag} \left( \begin{bmatrix} 1 & \cdots & 1 \\ \sigma_1^2 - \sigma_{n+1}^2 & \cdots & \sigma_n^2 - \sigma_{n+1}^2 \end{bmatrix} \right), \]
\[ D = \text{diag} \left( \begin{bmatrix} \sqrt{\sigma_1^2 + \sigma_{n+1}^2} & \cdots & \sqrt{\sigma_n^2 + \sigma_{n+1}^2} \end{bmatrix} \right). \]

Compared with (27), our (19) is simpler and more compact. Furthermore, (27) depends on the singular values and right singular vectors of both $A$ and $[A \ b]$. In contrast, (19) involves only singular values and right singular vectors of $[A \ b]$. Therefore, the computational cost of the condition number by (19) is half of that by (27). Furthermore, the following example shows that the computed results by (19) can be more accurate than those by (27).

**A small example.** We construct a TLS problem with $\hat{\sigma}_n$ and $\sigma_{n+1}$ very close. We generate $A, b$ by $[A \ b] = \text{generateAb}(m, n, \alpha)$ (see Appendix) by taking $m = 15, n = 10, \alpha = 10^{-8}$.

\[
\begin{array}{cccc}
\sigma_{n+1}/\sigma_n & \sigma_{n+1}/\hat{\sigma}_n & \kappa_r'(14) & \kappa_r'(19) \\
0.608 & 1 - 1.49 \times 10^{-12} & - & 1.13 \times 10^9 \times 3.12 \times 10^6 \\
\end{array}
\]

In the table, $\sigma_{n+1}/\sigma_n$ and $\sigma_{n+1}/\hat{\sigma}_n$ denote the quotients of $\sigma_{n+1}$ over $\sigma_n$ and $\hat{\sigma}_n$, respectively. $\kappa_r'(14)$, $\kappa_r'(19)$ and $\kappa_r'(27)$ denote the computed $\kappa_r'(A, b)$ by calculating $\kappa_g(A, b)$ via (13), (19) and (27), respectively. $\sigma_{n+1}$ and $\hat{\sigma}_n$ being so close makes $A^T A - \sigma_{n+1}^2 I_n$ numerically singular and makes $\kappa_g'(14)$ unreliable completely, so the result of $\kappa_g'(14)$ is omitted.

We comment that $\kappa_g'(19)$ is reliable as, by the remark in Appendix and Theorem 6, $\kappa(V_1^T) = \alpha^{-1} = 10^8$. This means that computing $\kappa_g(A, b)$ via (19) amounts to solving a moderately ill-conditioned linear system. Furthermore, the right-hand side $S$ of the system can be constructed with high accuracy since $\sigma_{n+1}$ and $\sigma_i$ are not close: $\frac{\sigma_{n+1}}{\sigma_i} \leq \frac{\sigma_{n+1}}{\sigma_{n+1}} = 0.608, i = 1, 2, \ldots, n$. In contrast, $\kappa_r'(27)$ is inaccurate since computing $\kappa_g(A, b)$ via (27) involves the diagonal matrix $\hat{D}$ and the closeness of $\sigma_{n+1}$ (about 0.299) and $\hat{\sigma}_n$ makes its last diagonal entry both very large (about $10^{15}$) and very inaccurate in finite precision arithmetic.

**4 Straightforward bounds on the TLS condition number**

**4.1 Sharp lower and upper bounds based on SVD of $[A \ b]$**

In this subsection, we further improve our result in Theorem 5 from the viewpoint of computational cost. We will show that with the SVD
\[ U^T [A \ b] V = \text{diag} (\sigma_1, \ldots, \sigma_{n+1}) \]
we are capable of estimating $\kappa_g(A, b)$ accurately based on the singular values of $[A \ b]$ and the last row of $V$ without calculating $\| V_{11}^T S \|$, where $V_{11} = V(1 : n, 1 : n), S = \text{diag} ([s_1, \ldots, s_n]), s_i = \sqrt{\sigma_i^2 + \sigma_{n+1}^2}, i = 1, \ldots, n$, as defined in Theorem 5.
From now on we denote \( \alpha = \frac{1}{\sqrt{1+\|x\|^2}} \), which is always smaller than one for \( x \neq 0 \).

Keep (25) in mind and note that
\[
s_1 \leq s_2 \leq \cdots \leq s_n.
\]

We then get
\[
s_n = \sigma_n(V_{11}^T)\|S\| \leq \|V_{11}^{-T}S\| \leq \|V_{11}^{-T}||S\| = \alpha^{-1}s_n.
\]

Therefore, from Theorem 5 we get
\[
\kappa := \alpha^{-1}s_n \leq \kappa_g(A, b) \leq \bar{\kappa} := \alpha^{-2}s_n.
\]

So, if \( \alpha \approx 1 \), that is, \( V_{11} \) is nearly an orthogonal matrix, the lower and upper bounds in (28) must be tight.

More generally, for \( \alpha \) not small, say, \( \frac{1}{2} < \alpha < 1 \), we have \( \bar{\kappa} < 4s_n \) and \( \kappa > s_n \). So \( \underline{\kappa} < \bar{\kappa} < 4\underline{\kappa} \). Therefore, in this case, our lower and upper bounds on the condition number \( \kappa_g(A, b) \) are very tight and can estimate the condition number accurately by no more than four times.

In the following, we only need to discuss the case that \( \alpha \leq \frac{1}{2} \). It will appear that we can establish some lower bound \( \underline{\kappa} \) and upper bound \( \bar{\kappa} \) such that \( \underline{\kappa} < \bar{\kappa} < 4\underline{\kappa} \) still holds. As a result, together with the above, for any \( 0 < \alpha < 1 \), we can estimate \( \kappa_g(A, b) \) accurately.

**Lemma 2** \( V \) can be written as
\[
V = \begin{bmatrix}
V_{11} & \sqrt{1-\alpha^2} \, \bar{u}_n \\
\sqrt{1-\alpha^2} \, \bar{v}_n^T & -\alpha
\end{bmatrix},
\]
where \( \bar{u}_n \) and \( \bar{v}_n \) are the left and right singular vectors associated with the smallest singular value of \( V_{11} \).

**Proof.** Based on Theorem 3 we let
\[
V_{11} = \bar{U} \begin{bmatrix} I_{n-1} & \alpha \end{bmatrix} \bar{V}^T
\]
be the SVD of \( V_{11} \), where \( \bar{U} = [\bar{u}_1, \ldots, \bar{u}_n] \in \mathbb{R}^{n \times n}, \bar{V} = [\bar{v}_1, \ldots, \bar{v}_n] \in \mathbb{R}^{n \times n}, \) and \( \bar{U}^T \bar{U} = \bar{V}^T \bar{V} = I_n \). It is easily justified from (4) that \( |V(n+1, n+1)| = \alpha \). Without loss of generality, we assume \( V(n+1, n+1) = -\alpha \). Then, by the theorem in Section 4 of [11], we get
\[
V = \begin{bmatrix} \bar{U} & \alpha \end{bmatrix} \begin{bmatrix}
I_{n-1} & O_{n-1,1} & O_{n-1,1} \\
O_{1,n-1} & \alpha \sqrt{1-\alpha^2} & -\alpha \\
O_{1,n-1} & \sqrt{1-\alpha^2} & -\alpha
\end{bmatrix} \begin{bmatrix} \bar{V}^T \\
1
\end{bmatrix}
\]

\[
= \begin{bmatrix} \bar{U} \begin{bmatrix} I_{n-1} & \alpha \end{bmatrix} \bar{V}^T & \sqrt{1-\alpha^2} \bar{u}_n \end{bmatrix},
\]

the desired form of \( V \). \( \square \)
Following Lemma 2 and letting $[\beta_1, \ldots, \beta_n, -\alpha]$ be the last row of $V$, we have

$$\bar{v}_n^T = \frac{1}{\sqrt{1 - \alpha^2}}[\beta_1, \ldots, \beta_n].$$  \hspace{1cm} (29)$$

Noticing that $(\alpha^{-1}, \bar{u}_n, \bar{v}_n)$ is the largest singular triplet of $V_{11}^{-T}$, we denote by

$$V_{11}^{-T} = [\bar{u}_n, \bar{u}_1, \ldots, \bar{u}_{n-1}]$$

which is the SVD of $V_{11}^{-T}$. Then, by (29) we have

$$V_{11}^{-T} = \begin{bmatrix}
\alpha^{-1}
\frac{\beta_1}{\sqrt{1 - \alpha^2}} & \cdots & \frac{\beta_n}{\sqrt{1 - \alpha^2}}
\bar{v}_1(1) & \cdots & \bar{v}_1(n)
\vdots & \vdots & \vdots
\bar{v}_{n-1}(1) & \cdots & \bar{v}_{n-1}(n)
\end{bmatrix}
\begin{bmatrix}
\bar{u}_n + w_1, \ldots, \alpha^{-1} \frac{\beta_1}{\sqrt{1 - \alpha^2}} \bar{u}_n + w_n, \ldots, \alpha^{-1} \frac{\beta_n}{\sqrt{1 - \alpha^2}} \bar{u}_n + w_n
\end{bmatrix},$$

(30)

where $\bar{v}_i(k)$ denotes the $k$th component of $\bar{v}_i$, $w_k = \sum_{i=1}^{n-1} \bar{v}_i(k)\bar{u}_i$, $k = 1, \ldots, n$.

**Lemma 3** For given matrices $A_1, A_2 \in \mathbb{R}^{n \times n}$, if $A_1^T A_2 = O$, then

$$\frac{1}{2} (\|A_1\| + \|A_2\|) \leq \|A_1 + A_2\|.$$  \hspace{1cm} (31)$$

**Proof.** For an arbitrary vector $x \in \mathbb{R}^n$, from $(A_1 x)^T (A_2 x) = 0$ it follows that

$$\|A_1 x\|, \|A_2 x\| \leq \|A_1 x + A_2 x\|$$

and that

$$\|A_1\| = \max_{\|x\|=1} \|A_1 x\| \leq \max_{\|x\|=1} \|A_1 x + A_2 x\| = \|A_1 + A_2\|,$$

$$\|A_2\| = \max_{\|x\|=1} \|A_2 x\| \leq \max_{\|x\|=1} \|A_1 x + A_2 x\| = \|A_1 + A_2\|.$$  

So, we get the desired inequality. \hfill \Box

To prove the main results of this section, we need the following two propositions.

**Proposition 1** Let $[\beta_1, \ldots, \beta_n, -\alpha]$ be the last row of $V$, $V_{11} = V(1 : n, 1 : n)$ and $S = \text{diag}([\bar{s}_1, \ldots, \bar{s}_n])$, where $\bar{s}_1, \ldots, \bar{s}_n$ are arbitrary positive numbers and satisfy $0 < \bar{s}_1 \leq \bar{s}_2 \leq \cdots \leq \bar{s}_n$. Then

$$\mathcal{L} := \frac{1}{2} \left( \frac{\alpha^{-1} \sqrt{\beta_1^2 \bar{s}_1^2 + \cdots + \beta_n^2 \bar{s}_n^2}}{\sqrt{1 - \alpha^2}} + \frac{\sqrt{1 - \alpha^2 - \beta_1^2}}{\sqrt{1 - \alpha^2}} \bar{s}_n \right)$$

$$\leq \left\| V_{11}^{-T} S \right\| \leq \bar{c} := \frac{\alpha^{-1} \sqrt{\beta_1^2 \bar{s}_1^2 + \cdots + \beta_n^2 \bar{s}_n^2}}{\sqrt{1 - \alpha^2}} + \bar{s}_n.$$
Proof. Following (30), we get

\[ \begin{array}{rcl}
V_{11}^{-T} \tilde{S} &=& \left[ \frac{\alpha^{-1} \beta_1 \tilde{s}_1}{\sqrt{1 - \alpha^2}} \tilde{u}_n + \tilde{s}_1 w_1, \ldots, \frac{\alpha^{-1} \beta_k \tilde{s}_k}{\sqrt{1 - \alpha^2}} \tilde{u}_n + \tilde{s}_k w_k, \ldots, \frac{\alpha^{-1} \beta_n \tilde{s}_n}{\sqrt{1 - \alpha^2}} \tilde{u}_n + \tilde{s}_n w_n \right].
\end{array} \]

Define

\[ A_1 = \left[ \frac{\alpha^{-1} \beta_1 \tilde{s}_1}{\sqrt{1 - \alpha^2}} \tilde{u}_n, \ldots, \frac{\alpha^{-1} \beta_n \tilde{s}_n}{\sqrt{1 - \alpha^2}} \tilde{u}_n \right], \quad A_2 = [\tilde{s}_1 w_1, \ldots, \tilde{s}_n w_n]. \]

Then \( V_{11}^{-T} \tilde{S} = A_1 + A_2 \). Noticing that \( \tilde{u}_T n w_k = 0, \ k = 1, \ldots, n, \) we get

\[ A_1^T A_2 = O. \]

Thus, we have

\[ \frac{1}{2} (\|A_1\| + \|A_2\|) \leq \left\| V_{11}^{-T} \tilde{S} \right\| \leq \|A_1\| + \|A_2\|, \tag{32} \]

in which the left-hand side inequality follows from Lemma 3. Furthermore, noticing that

\[ A_1 = \frac{\alpha^{-1}}{\sqrt{1 - \alpha^2}} \tilde{u}_n [\beta_1 \tilde{s}_1, \ldots, \beta_n \tilde{s}_n] \]

and \( \|\tilde{u}_n\| = 1 \), we have

\[ \|A_1\| = \frac{\alpha^{-1}}{\sqrt{1 - \alpha^2}} \|[\beta_1 \tilde{s}_1, \ldots, \beta_n \tilde{s}_n]| = \frac{\alpha^{-1}}{\sqrt{1 - \alpha^2}} \sqrt{\beta_1^2 \tilde{s}_1^2 + \ldots + \beta_n^2 \tilde{s}_n^2}. \tag{33} \]

In the meantime, note that

\[ \|w_n\| = \sqrt{n-1} \sum_{i=1}^{n-1} \tilde{v}_i^2(n) = \sqrt{1 - \frac{\beta_n^2}{1 - \alpha^2}} = \sqrt{\frac{1 - \alpha^2 - \beta_n^2}{1 - \alpha^2}}, \]

\[ \|[w_1, \ldots, w_n]\| = \left\| \begin{bmatrix} \tilde{v}_1^T & \cdots & \tilde{v}_{n-1}^T \end{bmatrix} \right\| = 1, \]

and

\[ \|\tilde{S}\| = \tilde{s}_n. \]

From

\[ \|\tilde{s}_n w_n\| \leq \|A_2\| \leq \|[w_1, \ldots, w_n]\| \|\tilde{S}\| \]

we get

\[ \frac{\sqrt{1 - \alpha^2 - \beta_n^2}}{\sqrt{1 - \alpha^2}} \tilde{s}_n \leq \|A_2\| \leq \tilde{s}_n. \tag{34} \]

Combining (32), (33) and (34), we establish the desired inequality. \( \square \)
Proposition 2 Suppose that \(\alpha \leq \frac{1}{2}\). Then for \(c\) and \(\bar{c}\) in Proposition 1, we have
\[
c < \bar{c} < 4c.
\] (35)

Proof. If \(\frac{|\beta_n|}{\sqrt{1 - \alpha^2}} < \frac{\sqrt{3}}{2}\), then it is easy to verify that
\[
\frac{\sqrt{1 - \alpha^2 - \beta_n^2}}{\sqrt{1 - \alpha^2}} > \frac{1}{2}
\]
and
\[
c > \frac{1}{4} \bar{c}.
\]

Thus, (35) holds. If \(\frac{|\beta_n|}{\sqrt{1 - \alpha^2}} \geq \frac{\sqrt{3}}{2}\), then
\[
\alpha^{-1} \frac{|\beta_n|}{\sqrt{1 - \alpha^2}} > \frac{\sqrt{3}}{2} \alpha^{-1} > 1,
\]
so \(\alpha^{-1} \frac{|\beta_n|}{\sqrt{1 - \alpha^2}} s_n > \bar{s}_n\), from which and the definitions of \(\bar{c}\) and \(c\) it follows that
\[
\bar{c} < \frac{\alpha^{-1} \sqrt{\beta_1^2 s_1^2 + \ldots + \beta_n^2 s_n^2}}{\sqrt{1 - \alpha^2}} + \alpha^{-1} \frac{|\beta_n|}{\sqrt{1 - \alpha^2}} \bar{s}_n
\]
\[
\leq 2 \alpha^{-1} \frac{\sqrt{\beta_1^2 s_1^2 + \ldots + \beta_n^2 s_n^2}}{\sqrt{1 - \alpha^2}}
\]
\[
\leq 2 \alpha^{-1} \frac{\sqrt{\beta_1^2 s_1^2 + \ldots + \beta_n^2 s_n^2}}{\sqrt{1 - \alpha^2}} + 2 \sqrt{1 - \alpha^2 - \beta_n^2} \bar{s}_n = 4c.
\]

Thus, (35) still holds. \(\square\)

Now we are in a position to derive sharp bounds on \(\kappa_g(A, b)\).

Theorem 7 Let \([\beta_1, \ldots, \beta_n, -\alpha]\) be the last row of \(V\) and \(S = \text{diag}([s_1, \ldots, s_n])\), \(s_i = \sqrt{\sigma_i^2 + \sigma_{i+1}^2} / \sigma_i^2 - \sigma_{i+1}^2\), \(i = 1, \ldots, n\). Then
\[
\kappa := \frac{1}{2} \left( \frac{\alpha^{-2} \sqrt{\beta_1^2 s_1^2 + \ldots + \beta_n^2 s_n^2}}{\alpha^{-1} \sqrt{1 - \alpha^2}} + \frac{1}{\sqrt{1 - \alpha^2}} \alpha^{-1} s_n \right)
\]
\[
\leq \kappa_g(A, b) \leq \bar{\kappa} := \frac{\alpha^{-2} \sqrt{\beta_1^2 s_1^2 + \ldots + \beta_n^2 s_n^2}}{\alpha^{-1} \sqrt{1 - \alpha^2}} + \alpha^{-1} s_n.
\]

Moreover, if \(\alpha \leq \frac{1}{2}\), then
\[
\bar{\kappa} < 4 \kappa.
\]

Proof. Noticing that \(0 < s_1 \leq s_2 \leq \cdots \leq s_n\) and using Proposition 1 we have
\[
\frac{1}{2} \left( \frac{\alpha^{-1} \sqrt{\beta_1^2 s_1^2 + \ldots + \beta_n^2 s_n^2}}{\alpha^{-1} \sqrt{1 - \alpha^2}} + \frac{1}{\sqrt{1 - \alpha^2}} \alpha^{-1} s_n \right)
\]
\[
\leq \left\| V_1^T S \right\| \leq \frac{\alpha^{-1} \sqrt{\beta_1^2 s_1^2 + \ldots + \beta_n^2 s_n^2}}{\sqrt{1 - \alpha^2}} + s_n.
\]
By Theorem 5, we get the first part of the theorem. Furthermore, we have the second part of the theorem by Proposition 2.

A small example (Continued). From Theorem 7, we have

$$5.65 \times 10^8 \leq \kappa_g^r(A, b) \leq 1.13 \times 10^9.$$ 

The lower and upper bounds estimate $\kappa_g^r(19) = 1.13 \times 10^9$ accurately, as described in the second part of Theorem 7.

4.2 Lower and upper bounds based on a few of singular values of $A$ and $[A \ b]$

In [10], bounds on the condition number of the Tikhonov regularization solution are established based on a few singular values of $A$, where $A$ is the coefficient matrix of the least squares problem under consideration. This is particularly useful for large scale TLS problems since for them any formulas and bounds for the condition number involving all the singular values of $A$ and/or $[A \ b]$ are too costly to be computed. Such a bound can be obtained by computing only a few singular values of $A$ and/or $[A \ b]$.

In the following theorem, we establish similar results for the condition number of the TLS problem.

**Theorem 8** We have

$$\kappa_1 \leq \kappa_g(A, b) \leq \bar{\kappa}_1,$$

where

$$\kappa_1 = \frac{\sqrt{1 + \|x\|^2} \sqrt{\hat{\sigma}_{n-1}^2 + \sigma_{n+1}^2}}{\hat{\sigma}_{n-1}^2 - \sigma_{n+1}^2}, \quad \bar{\kappa}_1 = \frac{\sqrt{1 + \|x\|^2} \sqrt{\sigma_n^2 + \sigma_{n+1}^2}}{\sigma_n^2 - \sigma_{n+1}^2}.$$

**Proof.** Denoting

$$M = (A^T A - \sigma_{n+1}^2 I_n)^{-1} ((\|x\|^2 + 1) A^T A + \|r\|^2 I_n) (A^T A - \sigma_{n+1}^2 I_n)^{-1},$$

from (17) we have

$$KK^T = M - 2\sigma_{n+1}^2 (A^T A - \sigma_{n+1}^2 I_n)^{-1} xx^T (A^T A - \sigma_{n+1}^2 I_n)^{-1}.$$ 

Here and hereafter, $\lambda_i(M)$ denotes the $i$th largest eigenvalue of $M$, where $M$ is an arbitrary symmetric matrix. By the Courant-Fischer theorem [14] p.182, from (38) we get

$$\lambda_2(M) \leq \lambda_1(KK^T).$$

Furthermore, since $2\sigma_{n+1}^2 (A^T A - \sigma_{n+1}^2 I_n)^{-1} xx^T (A^T A - \sigma_{n+1}^2 I_n)^{-1}$ is nonnegative definite, the following inequality holds

$$\lambda_1(KK^T) \leq \lambda_1(M).$$

Collecting (39) and (40) and based on (14), we have

$$\sqrt{\lambda_2(M)} \leq \kappa_g(A, b) \leq \sqrt{\lambda_1(M)}.$$
It is easy to verify that the set
\[
\left\{ \left( \frac{\|x\|^2 + 1}{\hat{\sigma}_j^2 - \sigma_{n+1}^2} \right)^{\hat{\sigma}_j^2} + \frac{\|r\|^2}{(\hat{\sigma}_j^2 - \sigma_{n+1}^2)^2} \right\}_{j=1}^{\infty}
\]
consists of all the eigenvalues of \( M \). We define the function
\[
f(\sigma) = \left( \frac{\|x\|^2 + 1}{\sigma - \sigma_{n+1}^2} \right)^{\hat{\sigma}_1^2 - \sigma_{n+1}^2 + 1}, \sigma > \sigma_{n+1},
\]
and differentiate it to get
\[
f'(\sigma) = -2\sigma^3 \left( \frac{\|x\|^2 + 1}{\sigma - \sigma_{n+1}^2} \right) - 2\sigma \left( \frac{\|x\|^2 + 1}{\sigma - \sigma_{n+1}^2} \right)^2.
\]
It is seen that \( f'(\sigma) < 0 \) and \( f(\sigma) \) is decreasing in the interval \((\sigma_{n+1}, \infty)\). Thus, we get
\[
\lambda_1(M) = \left( \frac{\|x\|^2 + 1}{\hat{\sigma}_1^2 - \sigma_{n+1}^2} \right)^{\hat{\sigma}_1^2 - \sigma_{n+1}^2 + 1}, \lambda_2(M) = \left( \frac{\|x\|^2 + 1}{\hat{\sigma}_1^2 - \sigma_{n+1}^2} \right)^{\hat{\sigma}_1^2 - \sigma_{n+1}^2 - 1}
\]
and
\[
\sqrt{\frac{\|x\|^2 + 1}{\hat{\sigma}_1^2 - \sigma_{n+1}^2}} \leq \kappa_g(A, b) \leq \sqrt{\frac{\|x\|^2 + 1}{\hat{\sigma}_1^2 - \sigma_{n+1}^2}}.
\]
Noticing that \( \frac{\|r\|^2}{1 + \|x\|^2} = \sigma_{n+1}^2 \), we complete the proof.

**Remark.** In Corollary 1 of [1], the authors prove that
\[
\kappa_g(A, b) \leq \sqrt{1 + \|x\|^2} \sqrt{\sigma_1^2 + \sigma_{n+1}^2}.
\]
Since \( \hat{\sigma}_n \leq \hat{\sigma}_1 \leq \sigma_1 \), we get
\[
\bar{\kappa}_1 \leq \sqrt{1 + \|x\|^2} \sqrt{\sigma_1^2 + \sigma_{n+1}^2} \leq \sqrt{1 + \|x\|^2} \sqrt{\sigma_1^2 + \sigma_{n+1}^2}.
\]
Therefore, our \( \bar{\kappa}_1 \) in [37] is sharper than the above upper bound.

It is seen that the lower and upper bounds on \( \kappa_g(A, b) \) in Theorem 8 are marginally different provided that \( \hat{\sigma}_n \) and \( \hat{\sigma}_{n-1} \) are close. This means that in this case both bounds are very tight. For the case that \( \hat{\sigma}_n \) and \( \hat{\sigma}_{n-1} \) are not close, we next give a new lower bound that can be better than that in Theorem 8.

**Theorem 9** It holds that
\[
\kappa_2 \leq \kappa_g(A, b) \leq \bar{\kappa}_1,
\]
where \( \bar{\kappa}_1 \) is defined as in Theorem 8 and
\[
\kappa_2 = \sqrt{\frac{1 + \|x\|^2}{\hat{\sigma}_n^2 - \sigma_{n+1}^2}}.
\]
Moreover, when \( \hat{\sigma}_{n-1} \geq \sigma_{n+1} + \sqrt{\sigma_n^2 - \sigma_{n+1}^2} \), we have
\[
\kappa_1 \leq \kappa_2.
\]

**Proof.** Denote \( P = A^T A - \sigma_{n+1}^2 I_n \). From [20], we have
\[
\frac{1}{\|x\|^2 + 1} KK^T = P^{-1} + 2\sigma_{n+1}^2 P^{-1} \left( I_n - \frac{xx^T}{1 + \|x\|^2} \right) P^{-1}.
\]
Noticing the second term in the right-hand side of the above relation is positive definite, we have
\[
(||x||^2 + 1) \lambda_1(P^{-1}) \leq \lambda_1(KK^T),
\]
that is,
\[
\frac{\|x\|^2 + 1}{\hat{\sigma}_n^2 - \sigma_{n+1}^2} \leq \kappa_g^2(A, b).
\]
Thus, the first part of the theorem is obtained.

The second part of the theorem is proved by noting
\[
\frac{\hat{\sigma}_{n-1}^2 + \sigma_{n+1}^2}{\hat{\sigma}_{n-1}^2 - \sigma_{n+1}^2} < \frac{1}{\sigma_{n-1} - \sigma_{n+1}} \leq \frac{1}{\sqrt{\hat{\sigma}_n^2 - \sigma_{n+1}^2}}
\]
under the assumption that \( \hat{\sigma}_{n-1} - \sigma_{n+1} \geq \sqrt{\hat{\sigma}_n^2 - \sigma_{n+1}^2} \).

**Remark 1.** At first glance, the assumption in the second part of the theorem seems not so direct but we can justify that it indeed implies that \( \hat{\sigma}_n \) and \( \hat{\sigma}_{n-1} \) are not close. Actually, we can verify that the second part of Theorem [9] holds under a slightly stronger but much simpler condition that
\[
\hat{\sigma}_{n-1} \geq 2\hat{\sigma}_n.
\]

**Remark 2.** From
\[
\bar{\kappa}_1 = \sqrt{\frac{\sigma_n^2 + \sigma_{n+1}^2}{\sigma_n^2 - \sigma_{n+1}^2}} = \sqrt{\frac{1 + \sigma_{n+1}^2}{1 - \sigma_{n+1}^2}} \bar{\kappa}_2 = \frac{\sigma_n^2 + \sigma_{n+1}^2}{\sqrt{\sigma_n^2 - \sigma_{n+1}^2}} \sqrt{\frac{1 + \sigma_{n+1}^2}{1 - \sigma_{n+1}^2}},
\]
it is seen that \( \frac{\bar{\kappa}_1}{\bar{\kappa}_2} > 1 \) provided \( \sigma_{n+1} > 0 \). Only for \( \sigma_{n+1} = 0 \), \( \bar{\kappa}_1 = \bar{\kappa}_2 \) holds. At this time, \( b \in \mathcal{R}(A) \) and \( r = 0 \).

We observe that the bounds on \( \kappa_g(A, b) \) in Theorem [9] are tight when \( \frac{\sigma_{n+1}}{\sigma_n} \) is small, compared with one. On the other hand, once \( \frac{\sigma_{n+1}}{\sigma_n} \) is not small, these bounds may not be tight. For this case, we will present new bounds that may better estimate \( \kappa_g(A, b) \).

The proof of the following theorem depends strongly on Propositions [1] and [2].

**Theorem 10** Assume that \( \alpha \leq \frac{1}{2} \). Denote \( \rho = \frac{\sigma_{n+1}}{\sigma_n} \). Then
\[
\kappa_2 := \sqrt{\frac{1 + \|x\|^2}{\sigma_n^2 - \sigma_{n+1}^2}} \leq \kappa_g(A, b) \quad < \quad \bar{\kappa}_2 := \sqrt{\frac{1 + 3\rho^2}{1 - \rho^2}} \sqrt{\frac{1 + \|x\|^2}{\sigma_n^2 - \sigma_{n+1}^2}} \quad (41)
\]
15
Proof. Based on Theorem [9] it suffices to prove the right-hand side of (41). From (20) and (23), we get

\[
\frac{1}{\|x\|^2 + 1} KK^T = P^{-1} + 2\sigma_{n+1}^2 P^{-1}\left(I_n - \frac{xx^T}{1 + \|x\|^2}\right) P^{-1},
\]

\[
= V_{11}^{-T} \Lambda^{-1} V_{11}^{-1} + 2\sigma_{n+1}^2 V_{11}^{-T} \Lambda^{-2} V_{11}^{-1} := P^{-1} + E, \tag{42}
\]

where \(P = A^T A - \sigma_{n+1}^2 I_n, \Lambda = \text{diag}([\alpha_1^2 - \sigma_{n+1}^2, \ldots, \sigma_n^2 - \sigma_{n+1}^2]).\) Denote

\[
D = \text{diag}([d_1, \ldots, d_n]), \quad d_i = \frac{\sigma_{n+1}}{\sigma_i^2 - \sigma_{n+1}^2}, i = 1, \ldots, n,
\]

\[
T = \text{diag}([t_1, \ldots, t_n]), \quad t_i = \frac{1}{\sqrt{\sigma_i^2 - \sigma_{n+1}^2}}, i = 1, \ldots, n.
\]

Then \(P^{-1} = \left(V_{11}^{-T} T \right) \left(T V_{11}^{-1} \right)\) and \(E = 2 \left(V_{11}^{-T} D \right) \left(D V_{11}^{-1} \right).\)

Note that \(0 < d_1 \leq d_2 \leq \cdots \leq d_n\) and \(0 < t_1 \leq t_2 \leq \cdots \leq t_n.\) Applying Proposition 1, we get

\[
\frac{1}{2} \left(\alpha^{-1} \sqrt{\beta_1^2 t_1^2 + \cdots + \beta_n^2 t_n^2} \sqrt{1 - \alpha^2 - \beta_n^2} d_n \right)
\]

\[
\leq \left\|V_{11}^{-T} D \right\| \leq \frac{\alpha^{-1} \sqrt{\beta_1^2 t_1^2 + \cdots + \beta_n^2 t_n^2}}{\sqrt{1 - \alpha^2}} + d_n \tag{43}
\]

and

\[
\frac{1}{2} \left(\alpha^{-1} \sqrt{\beta_1^2 t_1^2 + \cdots + \beta_n^2 t_n^2} \sqrt{1 - \alpha^2} t_n \right)
\]

\[
\leq \left\|V_{11}^{-T} T \right\| \leq \frac{\alpha^{-1} \sqrt{\beta_1^2 t_1^2 + \cdots + \beta_n^2 t_n^2}}{\sqrt{1 - \alpha^2}} + t_n,
\]

respectively, where \([\beta_1, \ldots, \beta_n, -\alpha]\) denotes the last row of \(V\) as before. Define \(k_n = \frac{d_n}{t_n} = \frac{\sigma_{n+1}}{\sqrt{\sigma_i^2 - \sigma_{n+1}^2}}.\) Then

\[
\frac{d_1}{t_1} \leq k_n, \ldots, \frac{d_{n-1}}{t_{n-1}} \leq k_n,
\]

\[
\frac{d_n}{t_n} = k_n.
\]

Thus, by (43) we have

\[
\frac{1}{\sqrt{2}} \left\|E \right\| \leq \left\|V_{11}^{-T} D \right\| \leq k_n \left(\alpha^{-1} \sqrt{\beta_1^2 t_1^2 + \cdots + \beta_n^2 t_n^2} + t_n \right). \tag{44}
\]

Note that for the lower and upper bounds on \(\left\|V_{11}^{-T} T \right\|\) above, by Proposition 2, it holds that

\[
\frac{\alpha^{-1} \sqrt{\beta_1^2 t_1^2 + \cdots + \beta_n^2 t_n^2}}{\sqrt{1 - \alpha^2}} + t_n < 2 \left(\frac{\alpha^{-1} \sqrt{\beta_1^2 t_1^2 + \cdots + \beta_n^2 t_n^2}}{\sqrt{1 - \alpha^2}} + \frac{\sqrt{1 - \alpha^2 - \beta_n^2} t_n}{\sqrt{1 - \alpha^2}} \right)
\]

\[
< 4 \left\|V_{11}^{-T} T \right\|. \tag{45}
\]
Based on (44) and (45), we derive that
\[ \frac{1}{\sqrt{2}} \|E\|^{\frac{1}{2}} < 4k_n \left\| V_1^{-TT} \right\| = 4k_n \| P^{-1} \|^{\frac{1}{2}} \]
and that
\[ \|E\| < 32k_n^2 \| P^{-1} \|. \quad (46) \]
Combining (46) and (42), we establish that
\[ \kappa_g(A, b) = \|K\| = \|KK^T\|^{\frac{1}{2}} < \sqrt{1 + 32k_n^2} \sqrt{1 + \|x\|^2} \| P^{-1} \|^{\frac{1}{2}} \]
\[ = \sqrt{1 + 31\rho^2} \sqrt{1 + \|x\|^2} \] \[ \sqrt{\frac{\hat{\sigma}^2_n}{\sigma_n^2 - \sigma_{n+1}^2}}. \]
So, the proof of the theorem is completed. \( \square \)

**Remark.** It is clear that the bounds in Theorem 10 are tight when \( \rho = \frac{\sigma_{n+1}}{\sigma_n} \) is small, compared with one. The result in this theorem is of particular importance in the case that \( \frac{\sigma_{n+1}}{\sigma_n} \) is close to one. Recall that the lower and upper bounds in Theorem 9 differ considerably when \( \frac{\sigma_{n+1}}{\sigma_n} \) is close to one. Theorem 10 tells us that, if only \( \frac{\sigma_{n+1}}{\sigma_n} \) is not so close to one, \( \kappa_g(A, b) \) should be close to the lower bound.

The improvement of \( \bar{\kappa}_2 \) to \( \bar{\kappa}_1 \) can be illustrated as follows. For \( \frac{\sigma_{n+1}}{\sigma_n} \) small, i.e., \( \sigma_{n+1} \) and \( \sigma_n \) not close, as an upper bound of \( \kappa_g^r(A, b) \),
\[ \bar{\kappa}_2 := \frac{\bar{\kappa}_2}{\|x\|} \| [A b] \|_F \]
\[ = \sqrt{1 + 31\rho^2} \sqrt{1 + \|x\|^2} \frac{\| [A b] \|_F}{\|x\|} \] \[ \sqrt{\frac{\hat{\sigma}^2_n}{\sigma_n^2 - \sigma_{n+1}^2}}. \]
is a moderate multiple of \( \frac{1}{\sqrt{\hat{\sigma}^2_n - \sigma_{n+1}^2}} \). In contrast,
\[ \bar{\kappa}_1 := \frac{\bar{\kappa}_1}{\|x\|} \| [A b] \|_F \]
\[ = \sqrt{1 + \|x\|^2} \frac{\sqrt{\sigma_n^2 + \sigma_{n+1}^2}}{\|x\|} \frac{\| [A b] \|_F}{\sigma_n^2 - \sigma_{n+1}^2} \]
\[ \approx \sqrt{\frac{\sigma_n^2 + \sigma_{n+1}^2}{\sigma_n^2 - \sigma_{n+1}^2}} \| [A b] \|_F \]
is a moderate multiple of \( \frac{1}{\sigma_n^2 - \sigma_{n+1}^2} \). The improvement of \( \bar{\kappa}_2^r \) over \( \bar{\kappa}_1^r \) becomes significant as \( \sigma_{n+1} \) and \( \hat{\sigma}_n \) are close. Similarly, \( \bar{\kappa}_2^r \) also improves the approximate condition number used in [2]:
\[ \bar{\kappa}_2^r := \frac{\hat{\sigma}_1}{\sigma_n - \sigma_{n+1}} = \frac{\hat{\sigma}_1(\hat{\sigma}_n + \sigma_{n+1})}{\hat{\sigma}_n^2 - \sigma_{n+1}^2}. \]

We will further illustrate the improvement by numerical experiments to be presented in Section 5.
5 Numerical experiments

We present numerical experiments to illustrate how tight the bounds in Theorems 9 and 10 are, and to compare the bounds with the related result in [2]. For a given TLS problem, the TLS solution is computed by (4). All experiments were run using Matlab 7.8.0 with the machine precision $\epsilon_{\text{mach}} = 2.22 \times 10^{-16}$ under the Microsoft Windows XP operating system.

Example 1. In this example, the TLS problem comes from [7]. Specifically, an $m \times (m - 2\omega)$ convolution matrix $\bar{T}$ is constructed to have the first column

$$t_{i,1} = \begin{cases} \sqrt{2\pi} \alpha \exp \left[ \frac{-(\omega - i + 1)^2}{2\alpha^2} \right] & i = 1, 2, \ldots, 2\omega + 1, \\ 0 & \text{otherwise}, \end{cases}$$

and the first row

$$t_{1,j} = \begin{cases} t_{1,1} & \text{if } j = 1, \\ 0 & \text{otherwise}, \end{cases}$$

where $\alpha = 1.25$ and $\omega = 8$. A Toeplitz matrix $A$ and a right-hand side vector $b$ are constructed as $A = \bar{T} + E$ and $b = \bar{g} + e$, where $\bar{g} = [1, \ldots, 1]^T$, $E$ is a random Toeplitz matrix with the same structure as $\bar{T}$ and $e$ is a random vector. The entries in $E$ and $e$ are generated randomly from a normal distribution with mean zero and variance one, and scaled so that

$$\|e\| = \gamma \|\bar{g}\|, \quad \|E\| = \gamma \|\bar{T}\|, \quad \gamma = 0.001.$$

Table 1:

| $m$ | $\sigma_{n+1}/\sigma_n$ | $\hat{\sigma}_{n+1}/\hat{\sigma}_n$ | $\kappa_i^r(A, b)$ | $\bar{\kappa}_2^r$ | $\bar{\kappa}_1^r$ | $\bar{\kappa}_{[2]}^r$ |
|-----|-------------------|-------------------|-------------------|-------------------|-------------------|-------------------|
| 100 | 0.981             | 1 - 7.85 \times 10^{-7} | 7.70 \times 10^7   | 7.04 \times 10^7   | 2.01 \times 10^{10}| 7.94 \times 10^{11}|
| 300 | 0.995             | 1 - 2.05 \times 10^{-10} | 1.40 \times 10^8   | 1.26 \times 10^8   | 6.90 \times 10^{10}| 8.83 \times 10^{11}|
| 500 | 0.998             | 1 - 5.66 \times 10^{-13} | 9.01 \times 10^9   | 7.89 \times 10^9   | 6.56 \times 10^{10}| 3.32 \times 10^{11}|

In the table,

$$\kappa_i^r = \frac{\bar{k}_2}{\|x\|} \|[A \ b]\|_F, \quad \bar{\kappa}_2^r = \frac{\bar{k}_2}{\|x\|} \|[A \ b]\|_F, \quad \bar{\kappa}_1^r = \frac{\bar{k}_1}{\|x\|} \|[A \ b]\|_F,$$

see Theorems 10 and 9 respectively. We calculate the approximate condition number used in [2]:

$$\bar{\kappa}_{[2]}^r = \frac{\hat{\sigma}_1}{\hat{\sigma}_n - \sigma_{n+1}}.$$

As indicated by the table, all the given TLS problems are similar in that $\sigma_{n+1}$ and $\hat{\sigma}_n$ are close but $\sigma_{n+1}$ and $\sigma_n$ are not so close. As estimates of $\kappa_i^r(A, b)$, the lower bounds $\kappa_i^r$ are very accurate, and the upper bounds $\bar{\kappa}_i^r$ improve the corresponding $\bar{\kappa}_i^r$ and $\bar{\kappa}_{[2]}^r$ significantly by one or two orders.
Example 2. In this example, the TLS problems are generated by the function described in Appendix. For given \( m, n \) and \( \alpha, A \) and \( b \) are generated by

\[
[A \ b] = \text{generateAbo}(m, n, \alpha).
\]

A different \( \alpha \) gives rise to a different TLS problem with different properties. As \( \alpha \) becomes smaller, \( \sigma_{n+1} \) and \( \hat{\sigma}_n \) become closer, so that the TLS problem becomes worse conditioned. For each of the TLS problems, we calculate the same quantities as those in Example 1 and list them in Table 2 in which the first set of data is for \((m, n) = (500, 350)\) and the second set is for \((m, n) = (1000, 750)\).

\[
\begin{array}{|c|c|c|c|c|c|c|}
\hline
\alpha & \sigma_{n+1}/\sigma_n & \sigma_{n+1}/\hat{\sigma}_n & \kappa_g^r(A, b) & \bar{\kappa}_2^r & \hat{\kappa}_2^r & \kappa_2^r \hat{\kappa}_2^2 \\
\hline
10^{-2} & 0.953 & 1 - 3.05 \times 10^{-4} & 2.55 \times 10^4 & 8.98 \times 10^9 & 1.60 \times 10^6 & 5.14 \times 10^6 & 6.29 \times 10^8 \\
10^{-3} & 0.980 & 1 - 3.16 \times 10^{-6} & 2.01 \times 10^5 & 8.75 \times 10^4 & 2.42 \times 10^6 & 4.92 \times 10^7 & 6.03 \times 10^7 \\
10^{-5} & 0.953 & 1 - 2.77 \times 10^{-10} & 1.97 \times 10^7 & 9.78 \times 10^6 & 1.74 \times 10^8 & 5.87 \times 10^{11} & 7.20 \times 10^{11} \\
10^{-7} & 0.966 & 1 - 1.80 \times 10^{-14} & 3.28 \times 10^9 & 1.12 \times 10^8 & 2.38 \times 10^{10} & 8.38 \times 10^{15} & 1.02 \times 10^{16} \\
10^{-2} & 0.983 & 1 - 2.78 \times 10^{-4} & 6.76 \times 10^4 & 1.65 \times 10^9 & 4.97 \times 10^6 & 9.90 \times 10^6 & 1.21 \times 10^8 \\
10^{-3} & 0.978 & 1 - 1.95 \times 10^{-6} & 6.70 \times 10^5 & 1.93 \times 10^5 & 5.09 \times 10^6 & 1.38 \times 10^9 & 1.69 \times 10^8 \\
10^{-5} & 0.968 & 1 - 3.01 \times 10^{-10} & 4.33 \times 10^7 & 1.60 \times 10^7 & 3.52 \times 10^8 & 9.24 \times 10^{11} & 1.13 \times 10^{12} \\
10^{-7} & 0.993 & 1 - 3.82 \times 10^{-14} & 1.13 \times 10^{10} & 1.44 \times 10^9 & 7.02 \times 10^{10} & 7.38 \times 10^{15} & 9.03 \times 10^{15} \\
\hline
\end{array}
\]

We can see from the table that, for \( \alpha = 10^{-2} \) in which \( \hat{\sigma}_n \) and \( \sigma_{n+1} \) are not very close, \( \bar{\kappa}_1^r \) and \( \hat{\kappa}_2^r \) are very tight and they estimate \( \kappa_g^r(A, b) \) quite accurately; for \( \alpha \leq 10^{-3} \), \( \hat{\sigma}_n \) and \( \sigma_{n+1} \) become closer with decreasing \( \alpha \), \( \bar{\kappa}_1^r \) and \( \hat{\kappa}_2^r \) estimate \( \kappa_g^r(A, b) \) increasingly more poorly. In contrast, however, for all the cases, since \( \sigma_n \) and \( \sigma_{n+1} \) are not so close, \( \bar{\kappa}_2^r \) and \( \hat{\kappa}_2^r \) estimate \( \kappa_g^r(A, b) \) accurately. Particularly, for \( \alpha \leq 10^{-5} \), \( \bar{\kappa}_2^r \) improves \( \hat{\kappa}_1^r \) and \( \hat{\kappa}_2^r \) very considerably by several orders.

6 Concluding Remarks

In the paper, we have mainly studied the condition number of the TLS problem and its lower and upper bounds that can be numerically computed cheaply. For the TLS condition number, we have derived a new closed formula. For a computational purpose, we can use it to compute the condition number more accurately. We have derived a few bounds, which are quite sharp and can be calculated cheaply. We have confirmed our results numerically and demonstrated the tightness of our bounds by numerical experiments.

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A Codes for generating tested TLS problems

The following codes produce an \( m \times (n+1) \) matrix \([A\ b]\), which has the SVD \([A\ b] = U\Sigma V^T\) with \( V(n+1, n+1) = -\alpha \), where \( 0 < \alpha < 1 \).

\[
[A\ b] = \text{generateAb}(m, n, \alpha)
\]

\%

\( m, n : \) two given positive integers with \( m \geq n \)

\( \% \alpha : \) a given positive number with \( 0 < \alpha < 1 \)

Generate \( \hat{V} ; \% \) a random orthogonal matrix of order \( n \)

\( V = \text{generateV}(n, \hat{V}, \alpha) \);

\( B = \text{rand}(m, n+1); \% \) the Matlab function \( \text{rand}(\) \)

\( [U, \Sigma, \hat{V}] = \text{svd}(B, 0); \% \) the Matlab function \( \text{svd}(\) \)

\( [A\ b] = U * \Sigma * V^T \)

The subfunction \( \text{generateV}(\) \) is shown as follows. It is used to produce an \( (n+1) \times (n+1) \) orthogonal matrix \( V \) with \( V(n+1, n+1) = -\alpha \), where \( 0 < \alpha < 1 \). The idea of construction comes from Lemma 2.

\[
[V] = \text{generateV}(n, \hat{V}, \alpha)
\]

\%

\( n : \) a given positive integer

\( \% \hat{V} : \) a given orthogonal matrix of order \( n \)

\( \% \alpha : \) a given positive number with \( 0 < \alpha < 1 \)

partition \( \hat{V} = [\hat{v}_1, \ldots, \hat{v}_n]; \)

generate \( U = [u_1, \ldots, u_n]; \% \) a random orthogonal matrix of order \( n \)

\( V_{11} = [u_1, \ldots, u_{n-1}][\hat{v}_1, \ldots, \hat{v}_{n-1}]^T + \alpha u_n \hat{v}_n^T; \)

\( V = \begin{bmatrix}
V_{11} & \sqrt{1-\alpha^2} u_n \\
\sqrt{1-\alpha^2} \hat{v}_n^T & -\alpha
\end{bmatrix} \)

Remark. Lemma 4.3 in [5] gives

\[
\frac{|\hat{u}_n^T b|}{2(\tilde{\sigma}_n - \sigma_{n+1})} \leq \|x\| \leq \frac{\|b\|}{\tilde{\sigma}_n - \sigma_{n+1}}.
\]

Equivalently, it holds that

\[
\frac{|\hat{u}_n^T b|}{2\|x\|} \leq \tilde{\sigma}_n - \sigma_{n+1} \leq \frac{\|b\|}{\|x\|}, \quad (47)
\]

where it is supposed that \( x \neq 0 \). Note that \( V(n+1, n+1) = -\alpha \) and \( \alpha = \frac{1}{\sqrt{1+\|x\|}} \). From \( (47) \) we see that a small \( \alpha \) implies that \( \tilde{\sigma}_n \) and \( \sigma_{n+1} \) are close in some sense.

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