On condition numbers of the total least squares problem with linear equality constraint

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Abstract This paper is devoted to condition numbers of the total least squares problem with linear equality constraint (TLSE). With novel limit techniques, closed formulae for normwise, mixed and componentwise condition numbers of the TLSE problem are derived. Computable expressions and upper bounds for these condition numbers are also given to avoid the costly Kronecker product-based operations. The results unify the ones for the TLS problem. For TLSE problems with equilibratory input data, numerical experiments illustrate that normwise condition number-based estimate is sharp to evaluate the forward error of the solution, while for sparse and badly scaled matrices, mixed and componentwise condition numbers-based estimates are much tighter.

Keywords Total least squares problem with linear equality constraint · Weighted total least squares problem · Condition number · Perturbation analysis

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1 Introduction

In many data fitting and estimation problems, total least squares model (TLS) [34] is used to find a “best” fit to the overdetermined system \( Ax \approx b \), where \( A \in \mathbb{R}^{q \times n} (q > n) \) and \( b \in \mathbb{R}^q \) are contaminated by some noise. The model determines perturbations \( E \in \mathbb{R}^{q \times n} \) to the coefficient matrix \( A \) and \( f \in \mathbb{R}^q \) to the vector \( b \) such that

\[
\min_{E,f} \| [E \ f] \|_F, \quad \text{subject to} \quad (A + E)x = b + f, \tag{1.1}
\]

where \( \| \cdot \|_F \) denotes the Frobenius norm of a matrix. The TLS model was carefully proposed in 1901 [34]. However it was not extensively explored for a long time. In recent forty years, it has been widely applied in a broad class of scientific disciplines such as system identification [22], image processing [32,33], speech and audio processing [19,23], etc. A wide range of concern on TLS owes to Golub and Van Loan, who introduced the TLS model to the numerical linear algebra area in 1980 [14], and they developed an...
algorithm for solving the TLS problem through the singular value decomposition (SVD) of $[A \ b]$. When $A$ is large, a complete SVD will be very costly. One improvement is to compute a partial SVD based on Householder transformation [40] or Lanczos bidiagonalization introduced by Golub and Kahan [15]. Another improvement is based on the Rayleigh quotient iteration [3], or Gauss-Newton iteration [11,38]. Recently, a randomized algorithm [49] presented by Xie et al. in 2018 greatly reduces the computational time and still maintains good accuracy with very high probability. For a comprehensive reading about the TLS model, we refer to [30],[41],[42].

In 1992, Dowling et al. [10] studied the TLS model with linear equality constraint (TLSE):

$$\min_{E,f} \|E \ f\|_F, \quad \text{subject to} \quad (A + E)x = b + f, \quad Cx = d, \quad (1.2)$$

where $C \in \mathbb{R}^{p \times n}$ is of full row rank and $[C \ A]$ has full column rank. They proposed to solve it on the basis of QR and SVD matrix factorizations. Further investigations on problem TLSE were performed in [37], where iteration methods were derived based on the Euler-Lagrange theorem. Recently, Liu et al. [27] interpreted the TLSE solution as an approximation of the solution to an unconstrained weighted TLS (WTLS) problem, with a large weight assigned on the constraint, based on which a QR-based inverse iteration (QR-INV) method was presented.

For the sensitive analysis of a problem, the condition number measures the worst-case sensitivity of its solution to small perturbations in the input data. Combined with backward error estimate, an approximate upper bound can be derived for the forward error, that is, the difference between a perturbed solution and the exact solution. There are a lot of work studying condition numbers of the standard TLS problem, see [1,20,24,31,44,45,48,51,52]. As far as we know, condition numbers of the TLSE problem have not been studied in the literature. As a continuation of the previous work [27], in this paper we will investigate this issue.

In [36], by applying the method of Lagrange multipliers, Schaffrin proved that the TLSE solution satisfies the following generalized eigenvalue problem

$$\begin{bmatrix}
A^T A & A^T b & C^T \\
b^T A & b^T b & d^T \\
C & d & 0
\end{bmatrix}
\begin{bmatrix}
x \\
-1 \\
\lambda
\end{bmatrix}
= \nu^2_{\min}
\begin{bmatrix}
I_n \\
1 \\
0_p
\end{bmatrix}
\begin{bmatrix}
x \\
-1 \\
\lambda
\end{bmatrix},$$

where $\lambda$ is a quantity related to the vector of Lagrange multipliers, and $\nu^2_{\min}$ is the smallest generalized eigenvalue. Notice that the associated matrix $\text{diag}(I_{n+1},0_p)$ in the generalized eigenvalue problem is positive semidefinite, which causes difficulties in the perturbation analysis of the TLSE problem. To the best of our knowledge, there are no good results about perturbation theory of generalized eigenvalue problem $Mx = \mu N x$ with $N$ being positive semidefinite.

In [36], Rice gave a general theory of condition numbers. If $x = \psi(a)$ is continuous and Fréchet differentiable function mapping from $\mathbb{R}^d$ to $\mathbb{R}$, where $a$ is a parameter related to input data. For small perturbations $\delta a$, denote $\delta x = \psi(a + \delta a) - \psi(a)$, then according to [36], the relative normwise condition number of $\psi$ at $a$ is

$$\kappa_{\text{rel}}(\psi,a) := \lim_{\varepsilon \to 0} \sup_{\|\delta a\| \leq \varepsilon \|a\|} \frac{\|\delta x\|_2/\|x\|_2}{\|\delta a\|_2/\|a\|_2} = \frac{\|\psi'(a)\|_2}{\|a\|_2},$$

where $\psi(a) \neq 0$, $\psi'(a)$ denotes the Fréchet derivative [36] of $\psi$ at the point $a$. In [1,20,24,31,48,51,52], condition number of TLS problems are generally based on Rice’s theory.

Although a closed form TLSE solution with Moore-Penrose inverse operation was given in [27] (see [24]), it is not easy to get a simple $\psi$ to derive its Fréchet derivative of the TLSE solution. Fortunately, the TLSE solution can be approximated by an unconstrained WTLS solution in a limit sense [27], while the perturbation of the standard TLS problem is widely investigated. In the literature, there are many similar problems whose perturbation analysis is derived based on a limit technique, say for equality constrained least squares problem by Wei and De Pierro [35,46,47]; Liu and Wei [28]; for mixed least squares-total least squares problem by Zheng and Yang [53]. In this paper, we consider modifying the
Perturbation results in [12,20,24] to be accessible for our problem, and then using the limit technique to derive the first order perturbation result of the TLSE solution, from which closed formulae of normwise, mixed and componentwise condition numbers are derived.

The organization of this paper is as follows. In Section 2, we present some preliminary results about TLS and TLSE problems. The first order perturbation result for the TLS problem is investigated in Section 3. Moreover, the Kronecker-product-based normwise, mixed and componentwise condition number formulae for the TLSE problem are given. To make the formulae more computable, Kronecker-product-free upper bounds for the normwise, mixed, and componentwise condition numbers are presented in Section 4. The perturbation estimates and condition number formulae for the standard TLS problem can be recovered from our results. In Section 5, some numerical examples are provided to demonstrate that our upper bounds are tight. Some concluding remarks are given in Section 6.

Throughout the paper, \( \| \cdot \|_2 \) denotes the Euclidean vector or matrix norm, \( I_n, 0_n, 0_{m \times n} \) denote the \( n \times n \) identity matrix, \( n \times n \) zero matrix, and \( m \times n \) zero matrix, respectively. If subscripts are ignored, the sizes of identity and zero matrices are consistent with the context. For a matrix \( M \in \mathbb{R}^{m \times n}, M^T, M^\dagger, \sigma_j(M) \) denote the transpose, the Moore-Penrose inverse, the \( j \)-th largest singular value of \( M \), respectively. \( \text{vec}(M) \) is an operator, which stacks the columns of \( M \) one underneath the other. The Kronecker product of \( A \) and \( B \) is defined by \( A \otimes B = [a_{ij}B] \) and its property is listed as follows [16,21]:

\[
\text{vec}(AXB) = (B^T \otimes A)\text{vec}(X), \quad (A \otimes B)^T = A^T \otimes B^T.
\]

2 Preliminaries

In this section we first recall some well known results about TLS and TLSE problems [10,14]. In order to apply the TLS theory to analyze the perturbation of problem TLSE conveniently, we use \([L \ h]\) as the input data and write the TLS model as the following form:

\[
\min \| [E \ f] \|_F, \quad \text{s.t.} \quad (L + E)x = h + f,
\]  

(2.1)

where \( L \in \mathbb{R}^{m \times n}, h \in \mathbb{R}^m (m > n) \). Following [14], if the SVD [15] of \([L \ h]\) is given by

\[
[L \ h] = U\Sigma V^T = \sum_{i=1}^{n+1} \sigma_i u_i v_i^T, \quad \Sigma = \text{diag}(\sigma_1, \sigma_2, \ldots, \sigma_{n+1}),
\]  

(2.2)

where \( \sigma_1 = \sigma_1([L \ h]) \) and \( \sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_{n+1} > 0 \), then under the Golub-Van Loan's genericity condition [14]:

\[
\sigma_n(L) > \sigma_{n+1}([L \ h]) = \sigma_{n+1},
\]  

(2.3)

the right singular vector \( v_{n+1} \) contains a nonzero last component, from which the TLS solution is uniquely determined by normalizing the last component to \(-1\). Moreover the TLS solution satisfies the following augmented system

\[
\begin{bmatrix}
L^T & L^T h \\
L^T & L^T h
\end{bmatrix}
\begin{bmatrix}
x \\
-1
\end{bmatrix}
= \begin{bmatrix}
\sigma_{n+1}^2 x \\
-1
\end{bmatrix},
\]  

(2.4)

from which

\[
L^T r = \sigma_{n+1}^2 x, \quad \text{for} \quad r = Lx - h,
\]  

(2.5)

and the closed form of the TLS solution can be expressed by

\[
x_{tls} = (L^T L - \sigma_{n+1}^2 I_n)^{-1} L^T h.
\]  

(2.6)

Let \([L \ h]\) be perturbed to \([L + \Delta L \ h + \Delta h]\), where \( \| [\Delta L \ \Delta h] \|_F \) is sufficiently small such that the genericity condition still holds for the perturbed TLS problem, then for the unique solution \( \hat{x}_{tls} \) of the perturbed TLS problem, Zhou et al. [51] first made the first order perturbation estimate based on [20,24].
and gave the explicit expressions of condition numbers. Li and Jia [24] presented a new and simple closed form formula with different approach and proved that \( \Delta x = \tilde{x}_{\text{tls}} - x_{\text{tls}} \) satisfies

\[
\Delta x = K \text{vec}(|\Delta L \Delta h|) + O(|||\Delta L \Delta h||_2^2),
\]

where \( x = x_{\text{tls}} \) is the exact TLS solution, and with \( r = Lx - h, P = L^T L - \sigma_{n+1}^2 I_n \),

\[
K = K_{LJ} = P^{-1} \left( \left( \frac{2LT_{yy}^T}{\|r\|_2^2} - L^T \right) \left( |x^T - 1| \otimes I_m \right) - \left[ I_n \ 0_{n \times 1} \right] \otimes r^T \right).
\]

They also proved that this closed formula is equivalent to the one from Zhou et al. [51]. In the same year, Baboulin and Gratton derived another formula of \( K \) in [1]:

\[
K_{BG} = \left[ - (x^T \otimes D) - (r^T \otimes P^{-1}) I_{m,n} \right] D,
\]

where \( D = P^{-1}(L^T - \frac{2xx^T}{\|x\|_2^2}), \rho = (1 + \|x\|_2^2)^{1/2}, \) and \( I_{m,n} \) is a vec-permutation matrix such that vec(\( Z^T \)) = \( I_{m,n} \text{vec}(Z) \) for an arbitrary \( m \times n \) matrix \( Z \). In [48], Xie et al. proved that \( ||K_{BG}||_2 = ||K_{LJ}||_2 \) and the associated normwise condition numbers are equivalent. In [29], Liu et al. proved that

\[
K_{BG} = \left[ - (x^T \otimes D) - P^{-1}(I_n \otimes r^T) \right] D = K_{LJ}.
\]

For the TLSE problem [12], denote \( \tilde{A} = [A \ b], \tilde{C} = [C \ d] \). In [10], the QR-SVD procedure for computing the TLSE solution first factorizes \( \tilde{C}^T \) into the QR form:

\[
\tilde{C}^T = \tilde{Q} \tilde{R} = [\tilde{Q}_1 \quad \tilde{Q}_2] \begin{bmatrix} \tilde{R}_1 \\ 0 \end{bmatrix} = \tilde{Q}_1 \tilde{R}_1, \quad \text{with} \quad \tilde{Q}_1 \in \mathbb{R}^{(n+1) \times p}, \tilde{R}_1 \in \mathbb{R}^{p \times p},
\]

and then computes the SVD of \( \tilde{A} \tilde{Q}_2 \) as

\[
\tilde{A} \tilde{Q}_2 = \tilde{U} \Sigma \tilde{V}^T = \sum_{i=1}^{n-p+1} \tilde{\sigma}_i \tilde{u}_i \tilde{v}_i^T.
\]

If \( \tilde{Q}_2 \tilde{v}_{n-p+1} \) contains a nonzero last component, a TLSE solution \( x = x_{\text{tls}} \) is determined by normalizing the last component in \( \tilde{Q}_2 \tilde{v}_{n-p+1} \) to \(-1\), i.e.,

\[
\begin{bmatrix} x \\ -1 \end{bmatrix} = \rho \tilde{Q}_2 \tilde{v}_{n-p+1},
\]

where \( \rho = (1 + \|x\|_2^2)^{1/2} \) up to a factor \( \pm 1 \).

In [24], Liu et al. carried out further investigations on the uniqueness condition and the explicit closed form for the TLSE solution. For the thin QR factorization of \( \tilde{C}^T \):

\[
\tilde{C}^T = QR = [Q_1 \quad Q_2] \begin{bmatrix} R_1 \\ 0 \end{bmatrix} = Q_1 R_1,
\]

let \( x_C = C^d = Q_1 R_1^{-1} d \) be the minimum 2-norm solution to \( C x = d \) and set \( r_C = A x_C - b \). Note that \( Q_2 \) and the specific matrix

\[
\tilde{Q}_2 = \begin{bmatrix} Q_2 & \zeta x_C \\ 0 & -\zeta \end{bmatrix}, \quad \text{with} \quad \zeta = \left( 1 + \|x_C\|_2^2 \right)^{-1/2},
\]

have orthonormal columns and the spans of the columns are the null space of \( C \) and \( \tilde{C} \), respectively. Then under the genericity condition

\[
\sigma_{n-p}(AQ_2) := \sigma_{n-p} > \sigma_{n-p+1} := \sigma_{n-p+1}([AQ_2 \ \zeta r_C]),
\]
it was proved that there must be a nonzero last component in \( \tilde{Q}_2 \tilde{v}_{n-p+1} \), and hence the TLSE problem has a unique solution taking the form

\[
x_{\text{tlse}} = C^d - Q_2 S_{11}^{-1} Q_2^T A^T r_C = C^d_A d + K A^T b,
\]

where \( S_{11} = Q_2^T A Q_2 - \tilde{\sigma}_{n-p+1}^2 I_{n-p} \) and \( K = Q_2 S_{11}^{-1} Q_2^T \). Let \( P = I_n - C^d \), then it is obvious that

\[
C^d_A = (I_n - K A^T A) C^d, \quad K = (P(A^T A - \tilde{\sigma}_{n-p+1}^2 I_n) P)^T.
\]

With this, the TLSE solution can be regarded as the limit case of the solution to an unconstrained weighted TLS (WTLS) problem \([27]\):

\[
\min_{E, f} \| (\tilde{E} - \tilde{f}) \|_F \quad \text{subject to} \quad (L_\epsilon + \tilde{E}) x_\epsilon = h_\epsilon + \tilde{f},
\]

as \( \epsilon \) tends to zero, where

\[
L_\epsilon = W^{\epsilon -1}L = \left[ \begin{array}{c} \epsilon^{-1} C \\ A \end{array} \right], \quad h_\epsilon = W^{\epsilon -1}h = \left[ \begin{array}{c} \epsilon^{-1} d \\ b \end{array} \right], \quad \text{for} \quad W_\epsilon = \left[ \begin{array}{cc} \epsilon I_p & 0 \\ 0 & I_q \end{array} \right].
\]

Under the genericity assumption \([24, 15]\) and the assumption

\[
0 < 2 \epsilon^2 \| \tilde{C} \|_F^2 \| \tilde{A} \|_F^2 < \tilde{\sigma}_{n-p}^2 - \tilde{\sigma}_{n-p+1}^2,
\]

the WTLS solution is uniquely determined by \( x_\epsilon = (L_\epsilon^T L_\epsilon - \tilde{\sigma}_\epsilon^2 I_n)^{-1} L_\epsilon^T h_\epsilon \), where \( \tilde{\sigma}_\epsilon \) is the smallest singular value of \( [L_\epsilon \quad h_\epsilon] \) and

\[
\lim_{\epsilon \to 0^+} \tilde{\sigma}_\epsilon = \tilde{\sigma}_{n-p+1}, \quad \lim_{\epsilon \to 0^+} x_\epsilon = x_{\text{tlse}}.
\]

In \([27]\), Liu et al. presented the QR-based inverse iteration (QR-INV) for above weighting problem to get the TLSE solution, in which the initial QR factorization of \( [L_\epsilon \quad h_\epsilon] \) and the solution of two \((n + 1) \times (n + 1)\) triangular systems in each iteration loop are needed. This is costly when \( n \) increases. A recent study of the randomized TLS with Nyström scheme (NTLS) proposed by Xie et al. \([49]\) is also appropriate for solving above weighted TLS problem, and it is more adaptable than QR-INV in getting the minimum-norm solution, when \( \tilde{A} Q_2 \) has multiple smallest singular values, and the TLSE solution is not unique.

In the NTLS algorithm, the known or estimated rank is set as the regularization parameter, and the QR factorization and SVD are implemented on much smaller matrices. Most flops are spent on the matrix-matrix multiplications, which are the so-called BLAS-3 operations, resulting in potential efficiency of the algorithm. The algorithm is described as follows.

**Algorithm 2.1** \([49]\) Randomized algorithm for WTLS problem \([2.17]\) via Nyström scheme (NWTLS).

**Inputs:** \( C \in \mathbb{R}^{p \times n}, d \in \mathbb{R}^p, A \in \mathbb{R}^{q \times n}, b \in \mathbb{R}^q, \) weighting factor \( \epsilon \), and \( k < \ell (\ell \ll n), \) where \( \ell \) is the sample size.

**Output:** an approximated solution \( x_{\text{nwtls}} \) for the TLS problem.

1. Solve \((G^T G) X = \Omega \) where \( G = [L_\epsilon \quad h_\epsilon] \) is defined in \([2.18]\), and \( \Omega \) is an \((n + 1) \times \ell \) Gaussian matrix generated via Matlab command `randn(n + 1, \ell)`.
2. Compute the \((n + 1) \times \ell \) orthonormal matrix \( Q \) via QR factorization \( X = QR \).
3. Solve \((G^T G) Y = Q \), and form the \( \ell \times \ell \) matrix \( Z = Q^T Y \).
4. Perform the Cholesky factorization \( Z = J^T J \), and seek \( K \) by solving \( KJ = Y \).
5. Compute the SVD: \( K = V \Sigma U^T \), and form the solution \( x_{\text{nwtls}} = -v(1 : n)/v(n + 1), \) where \( v = V(:, 1) \).
Remark 1 Algorithm 2.1 is refined from the conventional randomized SVD (RSVD) of \((G^T G)^{-1}\). The RSVD \(13\) of a matrix \(M \in \mathbb{R}^{m \times (n+1)}\) usually starts from computing the orthonormal column basis of the projected matrix \(M \Omega\) with \(\Omega\) an \((n+1) \times \ell\) Gaussian matrix. The approximate SVD of \(M \approx QQ^T M\) is then obtained by computing the SVD of a smaller matrix \(Q^T M\). The RSVD algorithm approximates well large singular values and corresponding singular vectors \(18\) Thms.10.5,10.6], especially for the matrix with fast decay rate in its singular values.

In Algorithm 2.1 for the sake of stability, the system \((G^T G)X = H\) could be solved by computing the QR factorization of \(G\) and then solving two \(\ell \times \ell\) triangular systems, where the parameter \(\ell = k + t\) stands for the number of sampling, and \(k\) is the number of singular values and singular vectors we expect to compute. According to the proof of \(27\) Theorem 3.1, we know that \(G = [L_e \ h_e]\) has \(p\) singular values of order \(O(\epsilon^{-1})\) and \(n - p + 1\) singular values approximating those of \(\hat{A}Q_2\), therefore the matrix \((G^T G)^{-1}\) has at least \(n - p + 1\) dominant singular values much larger than those \(p\) singular values of \(O(\epsilon^2)\). In order for a higher accuracy of the algorithm, we can choose \(\ell = k + t\) with \(k = n - p + 1\), and the oversampling factor \(t\), say \(t = 5\). Moreover, if we can predict the number \(s\) of dominant singular values for \(\hat{A}Q_2\) that are much smaller than \(n - p + 1\), then we can choose the parameter \(k = s\) to reduce the computational cost.

3 Condition numbers of the TLSE problem

Condition numbers measure the sensitivity of the solution to the original data in problems, and they play an important role in numerical analysis. For the TLSE problem, let \(m = p + q\) and \(L, h\) be defined in (2.18), define the mapping \(\phi : \mathbb{R}^{m \times n} \times \mathbb{R}^m \rightarrow \mathbb{R}^n\) by
\[
\phi([L \ h]) = x = x_{\text{tlse}}.
\]

According to Rice’s theory of condition numbers \(36\), the Fréchet derivative \(\phi'([L \ h])\) such that
\[
\Delta x = \phi([L + \Delta L \ h + \Delta h]) - \phi([L \ h]) = \phi'([L \ h]) \cdot [\Delta L \ \Delta h] + O(||[\Delta L \ \Delta h]||_F^2)
\]
is necessary. As point out previously, there are some difficulties in constructing a simple expression \(x = \phi([L \ h])\) and computing \(\phi'([L \ h])\) directly. Instead, we can start from the differentiability of the weighted TLS solution \(x_e\) and then take the limits as the parameter \(\epsilon\) approaches zero to get the various condition numbers of the TLSE solution.

To this end, let \(L, h, L_e, h_e\) be defined in (2.18), and \(\Delta L, \Delta h\) are the perturbations of \(L\) and \(h\), respectively. The weight matrix \(W_e\) is not perturbed and therefore
\[
\tilde{L}_e = L_e + \Delta L_e = W_e^{-1}(L + \Delta L), \quad \tilde{h}_e = h_e + \Delta h_e = W_e^{-1}(h + \Delta h),
\]
where the norms \(||[\Delta L \ \Delta h]||_F, \|[\Delta L_e \ \Delta h_e]||_F\|\) of perturbations are sufficiently small such that perturbed TLS and WTLS problems have unique solutions \(\tilde{x}_{\text{tlse}}\) and \(\tilde{x}_e\), respectively. In the limit sense,
\[
\tilde{x}_{\text{tlse}} = \lim_{\epsilon \rightarrow 0^+} \tilde{x}_e.
\]

The following lemma is necessary in analyzing the first order perturbation analysis of the weighted TLS solution \(\tilde{x}_e\).

Lemma 3.1 For the TLS problem defined in (2.1), if the SVD of \([L \ h]\) is given by (2.2) and the genericity condition \(23\) still holds, then we can express the first order perturbation result in (2.7)-(2.9) as
\[
\Delta x = K \vec{\text{vec}}([\Delta L \ \Delta h]) + O(||[\Delta L \ \Delta h]||_F^2),
\]
where with \(P = L^T L - \sigma_{n+1}^2 I_n\) and \(G(x) = [x^T - 1] \otimes I_n\), the matrix \(K\) has the following equivalent forms
\[
K_{LJ} = P^{-1} (2\sigma_{n+1}^{-2} x u_{n+1}^T G(x) - L^T G(x) - \rho \sigma_{n+1} I_n \otimes u_{n+1}^T) \otimes I_n, \quad K_{BG} = \begin{bmatrix} (x^T \otimes D) - \rho \sigma_{n+1} P^{-1} (I_n \otimes u_{n+1}^T) \otimes D \end{bmatrix}.
\]
Here $D = P^{-1}(L^T - \frac{2\sigma_{n+1}}{\rho}r u_{n+1}^T)$ with $\rho = \sqrt{1 + \|x\|^2}$ up to a sign $\pm 1$. The sign is determined by the one of the $(n+1)$-th component of $v_{n+1}$, and the value of $\rho u_{n+1}$ is unique and independent of the sign.

**Proof** Note that in (2.8), \[ x_{-1} = \rho v_{n+1} \] for $\rho = \pm \sqrt{1 + \|x\|^2}$ and \[ r = L x - h = \rho |L | b | v_{n+1} = \rho \sigma_{n+1} u_{n+1}, \quad \|r\|_2 = \rho^2 \sigma_{n+1}, \] from which we observe that the value of $\rho u_{n+1}$ is uniquely determined by $r/\sigma_{n+1}$. Without loss of generality, hereafter we take $\rho = \sqrt{1 + \|x\|^2}$. Combining with (2.5), we have \[ \frac{2L^T r r^T}{\|r\|^2} = \frac{2\sigma_{n+1} x u_{n+1}^T}{\rho}. \]

By substituting the new expression of $r$ into (2.8) and (2.9), we complete the proof. \hfill \Box

**Lemma 3.2** Let $L, h, \tilde{\sigma}$ be defined in (2.10). Assume that the QR factorization of $C^T$ is given by (2.10), then \[ \lim_{\epsilon \to 0^+} \tilde{\sigma} = \tilde{\sigma}_{n+1} \] and \[ \frac{(L^T \sigma_{n+1} - \tilde{\sigma}_{n+1})^{-1}}{\rho} (C^T A^T A - \epsilon^2 \tilde{\sigma}_{n+1})^{-1} = Q S_{11}^{-1} Q T^T = K, \]

where $S_{11} = Q_T^T A^T AQ_2 - \tilde{\sigma}_{n+1}^{-2} I_{n-p}, C_A, K$ are the same as in (2.17).

**Proof** The limits of $\tilde{\sigma}$ and $(L^T \sigma_{n+1} - \tilde{\sigma}_{n+1})^{-1}$ are straightforward from the proof of Theorem 3.2 in [27], by replacing $\mu$ there with $\epsilon^{-1}$.

For the last equality, we notice that the QR factorization of $C^T$ in (2.10) gives \[ H_\epsilon := \epsilon^{-2} (L^T \sigma_{n+1} - \tilde{\sigma}_{n+1})^{-1} C = (C^T C + \epsilon^2 A^T A - \epsilon^2 \tilde{\sigma}_{n+1}^{-2} I_{n-p})^{-1} C^T \]

Set $Z = Q^T A^T A - \epsilon^2 \tilde{\sigma}_{n+1} I_{n-p}$, and partition $Z$ conformal with $RR^T$, then \[ H_\epsilon = Q \left[ R_1 R_1^T + \epsilon^2 Z_{12} Z_{12} \right]^{-1} Q T^T =: Q \left[ Y_\epsilon^{(1)} \right] \]

in which $Y_\epsilon^{(1)}, Y_\epsilon^{(2)}$ also satisfy \[ \begin{bmatrix} R_1 R_1^T + \epsilon^2 Z_{12} Z_{12} \\ Z_{12} \end{bmatrix} \begin{bmatrix} Y_\epsilon^{(1)} \\ Y_\epsilon^{(2)} \end{bmatrix} = \begin{bmatrix} R_1 \\ 0 \end{bmatrix}. \]

Note that as $\epsilon$ tends to zero, $Z_{22}$ tends to $S_{11}$ which is nonsingular. By block Gaussian transformations to eliminate $\epsilon^2 Z_{12}$ to zero, we obtain \[ \lim_{\epsilon \to 0^+} Y_\epsilon^{(1)} = \lim_{\epsilon \to 0^+} [R_1 R_1^T + \epsilon^2 (Z_{12} - Z_{12} Z_{12} Z_{12}^{-1} Z_{12})]^{-1} R_1 = R_1^{-T}, \]

Consequently,

\[ \lim_{\epsilon \to 0^+} H_\epsilon = Q R_1 R_1^{-T} - Q S_{11}^{-1} Q T^T = C_A, \]

leading to the desired result. \hfill \Box
Lemma 3.3 ([39]) Let an \( n \times k \) matrix \( X \) have full column rank \( k \), and \( X \) be partitioned as \( X = [X_1 \ X_2] \). Denote \( X_\epsilon = [X_1 \ \epsilon x_2] \), \( Y = X_1^T x_2 \) and \( \overline{X_2} = X_2 - X_1Y \). Then to each singular value \( s_1 \) of \( X_2 \), there is associated a unique singular value \( s_1^{(\epsilon)} \) of \( X_\epsilon \) which satisfies \( s_1^{(\epsilon)} = s_1 + O(\epsilon^2) \). If \( s_1 \) is simple and its right singular vector is denoted by \( v_1 \), then the corresponding right singular vector of \( X_\epsilon \) satisfies

\[
v_1^{(\epsilon)} = \left[ v_1 + O(\epsilon) \right] \\
\epsilon Y^T v_1 + O(\epsilon^2)
\]

and the corresponding left singular vector satisfies \( u_1^{(\epsilon)} = u_1 + O(\epsilon^2) \), where \( u_1 \) is the left singular vector of \( \overline{X_2} \). Moreover, to each singular value \( \tilde{s}_2 \) of \( \overline{X_2} \), there is associated a unique singular value \( s_2^{(\epsilon)} \) of \( X_\epsilon \) which satisfies \( s_2^{(\epsilon)} = \tilde{s}_2 + O(\epsilon^3) \). If \( \tilde{s}_2 \) is simple and its right singular vector is denoted by \( \tilde{v}_2 \), then the corresponding right singular vector of \( X_\epsilon \) satisfies

\[
v_2^{(\epsilon)} = \left[ -\epsilon Y \tilde{v}_2 + O(\epsilon^3) \right] \\
\tilde{v}_2 + O(\epsilon^2)
\]

and the corresponding left singular vector satisfies \( u_2^{(\epsilon)} = \tilde{u}_2 + O(\epsilon^2) \).

Theorem 3.4 Let \( C_A^T K_A L \), \( L \), \( h \) be defined by \((2.7)\) and \((2.18)\), respectively. Then with the notations in \((2.11)\) and \((2.14)\) and the genericity assumption \((2.15)\), \( x = x_{\text{tlse}} = \phi([L \ h]) \) is Fréchet differentiable in a neighborhood of \([L \ h] \) and the first order estimate of \( \Delta x \) is

\[
\Delta x = K_{L,h} v_1 \text{vec}([\Delta L \ \Delta h]) + O(||[\Delta L \ \Delta h]||_F^2)
\]

where \( G(x) = [x^T - 1] \otimes I_m \) for \( m = p + q \) and

\[
H_1 = 2\rho^{-2} K x^T - [C_A^T K A]^T, \quad H_2 = K([I_n \ 0_{n \times 1}] \otimes I^T),
\]

for \( \rho = \sqrt{1 + ||x||_2^2} \). \( I^T \) with \( r = Ax - b \).

Proof: We first perform the first order perturbation analysis of the weighted TLS problem in \((2.17)-(2.18)\). Define the mapping \( x_\epsilon = \phi([L_\epsilon \ h_\epsilon]) \). From Lemma 3.1, we have

\[
\Delta x_\epsilon \approx \phi^\prime([L_\epsilon \ h_\epsilon]) \cdot [\Delta L_\epsilon \ \Delta h_\epsilon] = K_\epsilon \text{vec}([\Delta L_\epsilon \ \Delta h_\epsilon]) = K_\epsilon Z_\epsilon \text{vec}([\Delta L \ \Delta h]),
\]

where \( Z_\epsilon = I_{n+1} \otimes W^{-1} \) and with \( P_\epsilon = L_\epsilon^T L_\epsilon - \sigma_\epsilon^2 I_n \), \( G(x_\epsilon) = [x_\epsilon^T - 1] \otimes I_n \), \( K_\epsilon = P_\epsilon^{-1} (2\sigma_\epsilon \rho_\epsilon^{-1} x_\epsilon u_\epsilon^T G(x_\epsilon) - L_\epsilon^T G(x_\epsilon) - \rho_\epsilon \sigma_\epsilon [I_n \ 0_{n \times 1}] \otimes u_\epsilon^T) \).

Here \( u_\epsilon \) is the left singular vector corresponding to the smallest nonzero singular value \( \tilde{\sigma}_\epsilon \) of \( L_\epsilon := [L_\epsilon \ h_\epsilon] \) and \( \rho_\epsilon = (1 + ||x_\epsilon||_2^2)^{1/2} \) up to a factor \( \pm 1 \).

By taking the limit in \((3.3)\), we conclude that \( x_{\text{tlse}} = \phi([L \ h]) \) satisfies

\[
\phi^\prime([L \ h]) = \lim_{\epsilon \to 0^+} K_\epsilon Z_\epsilon.
\]

To prove \( \phi^\prime([L \ h]) = K_{L,h} \), we note that for any matrix \( M_1 \in \mathbb{R}^{n \times m} \), \( M_2 \in \mathbb{R}^{n \times m} \),

\[
M_1 G(x_\epsilon) Z_\epsilon \text{vec}([\Delta L \ \Delta h]) = M_1 \left( [x_\epsilon^T - 1] \otimes W^{-1} \right) \text{vec}([\Delta L \ \Delta h]) = (M_1 W_\epsilon^{-1}) \left( [x_\epsilon^T - 1] \otimes I_m \right) \text{vec}([\Delta L \ \Delta h]),
\]

\[
M_2 \left( [I_n \ 0_{n \times 1}] \otimes u_\epsilon^T \right) Z_\epsilon \text{vec}([\Delta L \ \Delta h]) = M_2 \left( [I_n \ 0_{n \times 1}] \otimes (u_\epsilon^T W^{-1}) \right) \text{vec}([\Delta L \ \Delta h]).
\]
Then
\[
\phi'(\begin{bmatrix} L & h \end{bmatrix}) = \lim_{\epsilon \to 0^+} P_\epsilon^{-1} \left[ \left( 2\sigma_\epsilon \rho_\epsilon^{-1} x, u_\epsilon^T W_\epsilon^{-1} - L^T W_\epsilon^{-2} \right) G(x) - \rho_\epsilon \sigma_\epsilon [I_n \ 0_{n \times 1}] \otimes (u_\epsilon^T W_\epsilon^{-1}) \right].
\]

Here \( u_\epsilon \) is the right singular vector of \([L_\epsilon \ h_\epsilon]^T = [\epsilon^{-1} \tilde{C}^T \tilde{A}^T] \) or \( \tilde{Q}^T [\tilde{C}^T \ \epsilon \tilde{A}^T] \), corresponding to its smallest nonzero singular value, where \( \tilde{Q} \) is defined in (3.10). Take \( X_1 = \tilde{Q}^T \tilde{C}^T = [\tilde{R}_1 \ 0] \), \( X_2 = \tilde{Q}^T \tilde{A}^T \) in Lemma 3.3 we obtain
\[
u_\epsilon = \left[ -\epsilon \tilde{C}^T \tilde{A}^T \tilde{u} + O(\epsilon^3) \right],
\]
where \( \tilde{u} \) is the left singular vector of \( \tilde{A}^T \tilde{Q} \), corresponding to its smallest nonzero singular value and it is exactly \( \tilde{u}_{n-p+1} \) according to the SVD in (2.11).

Note that \( \tilde{u}_{n-p+1} \) has a close relation to the residual vector \( r \) by (2.11)-(2.12), as revealed below
\[
\rho \tilde{u}_{n-p+1} = \rho \tilde{A} \tilde{Q} \tilde{u}_{n-p+1} = \tilde{A} \begin{bmatrix} x \\ -1 \end{bmatrix} = r.
\]

Combining (3.3) with (2.20) and Lemma 3.2 and for the terms in \( \phi'(\begin{bmatrix} L & h \end{bmatrix}) \) we obtain
\[
\begin{aligned}
\lim_{\epsilon \to 0^+} 2\sigma_\epsilon \rho_\epsilon^{-1} P_\epsilon^{-1} x, u_\epsilon^T W_\epsilon^{-1} G(x) & = 2\tilde{u}_{n-p+1} \rho^{-1} K x \tilde{u}_{n-p+1} \left[ -\tilde{A} \tilde{C}^T \right] I_q G(x) = 2\rho^{-1} K x t^T G(x), \\
\lim_{\epsilon \to 0^+} P_\epsilon^{-1} L^T W_\epsilon^{-2} G(x) & = [\tilde{C}^T \tilde{A} \tilde{C}^T] G(x), \\
\lim_{\epsilon \to 0^+} \rho_\epsilon \sigma_\epsilon [I_n \ 0_{n \times 1}] \otimes (u_\epsilon^T W_\epsilon^{-1}) & = \rho \tilde{u}_{n-p+1} \mathcal{K} \left( [I_n \ 0_{n \times 1}] \otimes (\tilde{u}_{n-p+1} \left[ -\tilde{A} \tilde{C}^T \right] I_q) \right) = \mathcal{K} \left( [I_n \ 0_{n \times 1}] \otimes t^T \right).
\end{aligned}
\]

The assertion in the theorem then follows. \( \square \)

By applying the similar technique on (2.20), we can prove another form of the perturbation result. The result is listed below, in which \( \overline{K}_{L,h} \) is equivalent to \( K_{L,h} \).

**Theorem 3.5** With the notations in Theorem 3.4, the first order estimate of the TLSE solution \( x \) is
\[
\Delta x = \overline{K}_{L,h} \text{vec}(\left[ \Delta L \ \Delta h \right]) + O(\|\Delta L \ \Delta h\|_F^2)
\]
\[
= [(x^T \otimes H_1) - \overline{H}_2 - H_1 \left[ \text{vec}(\Delta L) \ \text{vec}(\Delta h) \right]] + O(\|\Delta L \ \Delta h\|_F^2),
\]
where \( \overline{H}_2 = \mathcal{K}(I_n \otimes t^T) \).

Let \( \alpha, \beta \) be positive numbers, for the data space \( \mathbb{R}^{m \times n} \times \mathbb{R}^m \), define the flexible norm
\[
\|E \ f\|_F = \sqrt{\alpha^2 \|E\|_F^2 + \beta^2 \|f\|_2^2},
\]
which is convenient to monitor the perturbations on \( E \) and \( f \). For instance, large values of \( \alpha \) (resp. \( \beta \)) enable to obtain condition number problems where mainly \( f \) (resp. \( E \)) is perturbed. The idea of using parameter to unify the perturbations and condition numbers was first proposed in [17], and then used or extended by [13],[20].
Definition 3.6 Let $[L \ h]$ be defined in (2.13), and $[\Delta L \ \Delta h]$ is the perturbation to $[L \ h]$. Denote $\Delta x = \phi([L \ h] + [\Delta L \ \Delta h]) - \phi([L \ h])$, and define the normwise, mixed and componentwise condition numbers as follows

$$\kappa_n = \lim_{\eta \to 0} \sup_{\eta} \left\{ \frac{\|\Delta x\|_2}{\eta \|x\|_2} : \|\Delta L\|_F \leq \eta \|[L \ h]\|_F \right\},$$

$$\kappa_m = \lim_{\eta \to 0} \sup_{\eta} \left\{ \frac{\|\Delta x\|_\infty}{\eta \|x\|_2} : \|\Delta L\|_\infty \leq \eta \|[L \ h]\|_\infty \right\},$$

$$\kappa_c = \lim_{\eta \to 0} \sup_{\eta} \left\{ \frac{\|\Delta x\|_\infty}{\eta \|x\|_\infty} : \|\Delta L\|_\infty \leq \eta \|[L \ h]\|_\infty \right\},$$

where $\cdot \mid \cdot$ denotes the componentwise absolute value, $Y \leq Z$ means $y_{ij} \leq z_{ij}$ for all $i,j$, and $\frac{Y}{Z}$ is the entrywise division defined by $\frac{Y}{Z} := \{\frac{y_{ij}}{z_{ij}}\}$ and $\frac{0}{0}$ is interpreted as zero if $\zeta = 0$ and infinity otherwise. The subscripts in $\kappa$ characterize the type of the condition numbers.

Write $x = \phi([L \ h])$ as $x = \psi(g) = \bar{\psi}(\bar{g})$ for $g = \mathrm{vec}([L \ h])$, $\bar{g} = \mathrm{vec}([\alpha L \ \beta h])$ and $g = (D \otimes I_m)\bar{g}$, in which $D = \text{diag}(\alpha^{-1}I_n, \beta^{-1})$. By following the concept and formula for the normwise condition number in [5,12,13], the condition number formulae take the following form

$$\kappa_n = \frac{\|\bar{\psi}(\bar{g})\|_2}{\|\psi(g)\|_2} = \frac{\|K_{\alpha,\beta}\|_2 \|[L \ h]\|_F}{\|x\|_2},$$

$$\kappa_m = \frac{\|\bar{\psi}(\bar{g})\|_\infty \cdot \|g\|_\infty}{\|\psi(g)\|_\infty} = \frac{\|K_{L,h}\| \cdot \|\psi(g)\|_\infty}{\|\psi(g)\|_\infty} = \frac{\|K_{L,h}\| \cdot \|x\|_\infty}{\|x\|_\infty},$$

$$\kappa_c = \frac{\|\bar{\psi}(\bar{g})\|_\infty}{\|\psi(g)\|_\infty} = \frac{\|K_{L,h}\| \cdot \|\psi(g)\|_\infty}{\|\psi(g)\|_\infty} = \frac{\|K_{L,h}\| \cdot \|x\|_\infty}{\|x\|_\infty},$$

in which $K_{L,h}, K_{L,h}$ are defined in Theorems 3.5 and 3.6, respectively, and $K_{\alpha,\beta} = K_{L,h}(D \otimes I_m)$.

4 Compact formula and upper bounds of condition numbers

Note that the explicit expression of three types of condition numbers all involve the Kronecker product, which makes the storage and computation very costly. We provide compact formula and upper bounds that are Kronecker-product free and computable.

For mixed and componentwise condition numbers, it is obvious that

$$\kappa_m \leq \frac{\|H_1((||L||_x + |h|) + [K]\|L_l^T|)_t\|_\infty}{\|x\|_\infty} =: \kappa_m^U,$$

and

$$\kappa_c \leq \frac{\|H_1((||L||_x + |h|) + [K]\|L_l^T|)_t\|_\infty}{\|x\|_\infty} =: \kappa_c^U.$$
Lemma 4.1 (6) Given matrices $V \in \mathbb{R}^{m\times n}$, $X \in \mathbb{R}^{n\times m}$, $Y \in \mathbb{R}^{n\times n}$ and vectors $s \in \mathbb{R}^n$, $t \in \mathbb{R}^m$, $u \in \mathbb{R}^m$ with two positive real numbers $\alpha$ and $\beta$, for the linear operator $l$ defined by

$$l(V, u) := -XVs + YV^T t + Xu,$$

its operator weighted spectral norm can be characterized by

$$\|l\|_{2,F} = \sup_{V\neq 0, u \neq 0} \frac{\|l(V, u)\|_2}{\|V\|_F \|u\|_F},$$

$$= \left\| \begin{vmatrix} -\frac{\|s\|_2}{\beta} X & \frac{\|t\|_2}{\alpha} Y \\ 0 & \frac{\|t\|_2}{\alpha} \end{vmatrix} \right\|_2 \left[ c_1 I_m - c_2 \frac{t \alpha}{\|t\|_2} \begin{array}{c} \beta \\ 0 \end{array} \frac{t \alpha}{\|t\|_2} \right],$$

$$\leq \left( \frac{\|s\|_2}{\beta} \|X\|_2 + \frac{\|t\|_2}{\alpha} \|Y\|_2 \right) \sqrt{\max\{1, \frac{\beta^2}{\alpha^2} + \frac{1}{\|s\|_2^2} \} + \frac{\beta}{\alpha}},$$

where $c_1 = \pm \sqrt{\frac{\beta^2}{\alpha^2} + \frac{1}{\|s\|_2^2}}$, $c_2 = c_1 \pm \frac{1}{\|s\|_2^2}$.

Proof. In (6), Diao proved the value of $\|l\|_{2,F}$ for $c_1 = c_1^0, c_2 = c_2^0$, where $c_1^0 = \sqrt{\frac{\beta^2}{\alpha^2} + \frac{1}{\|s\|_2^2}}$ and $c_2^0 = c_1^0 + \frac{1}{\|s\|_2^2}$. Let

$$Z = L \left[ -\frac{1}{\beta} \|s\|_2^2 X \quad \frac{\|t\|_2}{\alpha} Y \right], \quad M = \left[ c_1 I_m - c_2 \frac{t \alpha}{\|t\|_2} \begin{array}{c} \beta \\ 0 \end{array} \frac{t \alpha}{\|t\|_2} \right],$$

where $\|ZM\|_2 = \|ZMM^TZ^T\|_F^{1/2}$ with

$$MM^T = \begin{bmatrix} \left( \frac{\beta^2}{\alpha^2} + \frac{1}{\|s\|_2^2} \right) I_m & 0 \\ 0 & I_n \end{bmatrix} + \begin{bmatrix} 0 \\ \frac{st^T \|t\|_2 \|s\|_2}{\|t\|_2 \|s\|_2} \end{bmatrix} \begin{array}{c} \beta \\ \alpha \end{array}.$$

The matrix product $MM^T$ keeps the same for $c_1 = \pm c_1^0, c_2 = c_1^0 \pm \frac{1}{\|s\|_2^2}$, and $\|M\|_2$ has the upper bound

$$\|M\|_2 = \|MM^T\|_2 \leq \max\{1, \frac{\beta^2}{\alpha^2} + \frac{1}{\|s\|_2^2} \} + \frac{\beta}{\alpha}.$$

The assertion of the lemma then follows. \qed

Theorem 4.2 With the notations in Theorem 3.4, we have the compact expression for the normwise condition number

$$\kappa_n = \left\| \begin{vmatrix} -\frac{\|x\|_2}{\beta} H_1 & \frac{\|t\|_2 \|K\|_2}{\alpha} \\ 0 & \frac{\|t\|_2 \|K\|_2}{\alpha} \end{vmatrix} \right\|_2 \frac{\|l\|_F}{\|x\|_2},$$

where $c_1 = \pm \sqrt{\frac{\beta^2}{\alpha^2} + \frac{1}{\|x\|_2^2}}$, $c_2 = c_1 \pm \frac{1}{\|x\|_2^2}$. The upper bound of $\kappa_n$ is given by

$$\kappa_n^U = \left( \frac{\|x\|_2}{\beta} \|H_1\|_2 + \frac{\|t\|_2 \|K\|_2}{\alpha} \right) \times \frac{\|l\|_F}{\|x\|_2} \sqrt{\max\{1, \frac{\beta^2}{\alpha^2} + \frac{1}{\|x\|_2^2} \} + \frac{\beta}{\alpha}},$$

$$\leq \left( \frac{\|x\|_2}{\beta} (\|C_A^T\|_2 + \|K\|_2 \|A\|_2) + \left( \frac{\beta}{\alpha} + \frac{1}{\|x\|_2^2} \right) \|K\|_2 \|t\|_2 \right) \times \frac{\|l\|_F}{\|x\|_2} \sqrt{\max\{1, \frac{\beta^2}{\alpha^2} + \frac{1}{\|x\|_2^2} \} + \frac{\beta}{\alpha}}.$$
Proof By Theorem 3.3 and 4.1, we have
\[ \Delta r = K_{L,h} \Delta g = H_1(\Delta L x - \Delta h) - \kappa \Delta L^T t + O(||\Delta L \quad \Delta h||_F^2), \]
for \( \Delta g = \text{vec}(\Delta L \quad \Delta h) \). Ignore the high-order terms and in Lemma 4.1 set
\[ X = H_1, \quad V = -\Delta L, \quad Y = \mathcal{K}, \quad s = x, \quad u = -\Delta h, \quad t^T = [-r^T(\tilde{A}\tilde{C}^T) \quad r^T], \]
for \( r = Ax - b \), then from (4.2) and Lemma 4.1 we get the compact expression for \( ||K_{\alpha,\beta}||_2 \) as
\[
||K_{\alpha,\beta}||_2 = \left[ -\frac{\|x\|^2}{\beta} H_1 \frac{||t||_2}{\alpha} \mathcal{K} \right] \left[ c_1 I_n - c_2 \frac{tt^T}{||t||_2} \frac{\beta}{\alpha} \frac{tt^T}{||t||_2} ||x||_2 \right] ||x||_2,
\]
and the expression for \( \kappa_n \), which is bounded by
\[
\kappa_n \leq \left( \frac{\|x\|^2}{\beta} \|H_1\|_2 + \frac{||t||_2}{\alpha} ||\mathcal{K}||_2 \right) \frac{||L||_2}{\|x||_2} \sqrt{\max\{1, \frac{\beta^2}{\alpha^2} + \frac{1}{\|x||_2} \}} + \frac{\beta}{\alpha},
\]
where \( ||H_1||_2 \leq 2||t||_2 ||\mathcal{K}||_2/\rho + ||C_A^T||_2 + ||\mathcal{K} A^T||_2 \). The proof is then finished. \( \square \)

Remark 2 The upper bound \( \kappa_n^U \) involves the computation of \( ||C_A^T||_2, ||\mathcal{K} A^T||_2 \) and \( ||t||_2 \), which can be easily implemented from the intermediate results for solving the TLS problem. For example, for the matrix \( \mathcal{K} = Q_2 S_1^T Q_2^T \) with \( S_1 = (AQ_2)^T(AQ_2) - \tilde{\sigma}_{n-p+1}^2 I_{n-p} \), we note that \( (AQ_2)^T(AQ_2) \) is just the \((n-p) \times (n-p)\) principle submatrix of \( (AQ_2)^T(AQ_2) \) and hence
\[
S_{11} = (AQ_2)^T(AQ_2) - \tilde{\sigma}_{n-p+1}^2 I_{n-p} = [I_{n-p} 0] \begin{bmatrix} (\tilde{A}\tilde{Q}_2)^T(\tilde{A}\tilde{Q}_2) - \tilde{\sigma}_{n-p+1}^2 I_{n-p} \end{bmatrix} [I_{n-p} 0] = V_{11} S_{11},
\]
where \( V_{11} \) is the principal \((n-p) \times (n-p)\) submatrix of \( V \). Its inverse \( S_{11}^{-1} = V_{11}^{-1} S_{11}^{-1} \), where \( V_{11} \) can be cheaply computed based on the formula in [9 Lemma 1]. For the vector \( t \), we can formulate \( \tilde{C}_i^T \) based on the Grevill’s method [2 Chapter 7, Section 5] as
\[
\tilde{C}_i^T = \begin{bmatrix} (I_n - \omega^{-1} x_C x_C^T \tilde{C}_i^T) \tilde{C}_i^T \\ \omega^{-1} x_C^T \tilde{C}_i^T \end{bmatrix}, \quad \omega = 1 + \|x_C\|^2,
\]
where \( \tilde{C}_i^T \) can be easily obtained from the QR factorization of the matrix \( (b - A\tilde{C}) \).

Remark 3 As a check, we can recover the perturbation bound and condition numbers for the standard TLS problem, by setting \( C = \Delta C = 0 \) and \( d = \Delta d = 0 \) in Theorem 3.3. In this case, \( C_A^T = 0_{n \times p} \), \( \mathcal{K} = (A^T A - \sigma_{n+1}^2 I_{n+1})^{-1} =: P^{-1}, \quad t^T = [0_{1 \times p} \quad r^T], \)
where \( \sigma_{n+1} = \sigma_{n+1}(A \quad b) \), and by setting \( C = 0 \) and \( d = 0 \) in (2.4)-(2.5), we derive that \( A^T r = \sigma_{n+1}^2 x \) and \( \|r\|^2 = \sigma_{n+1}^2 \rho^2 \), from which \( \rho^{-2} x = \frac{A^T r}{\|r\|^2} \) and
\[
H_1 = \bar{P}^{-1}0_{n \times p} \quad 2\rho^{-2} x r^T - A^T = \bar{P}^{-1}0_{n \times p} - A^T H_0,
\]
with \( H_0 = I_q - 2x r^T \|r\|^2 \) being a Householder matrix, therefore \( K_{L,h} = 0_{n \times p} \quad K_{11s} \) with \( K_{11s} = K_{i1s} \) that is defined in (2.8). The absolute normwise condition number \( \kappa_n^{\text{abs}} = ||K_{L,h}||_2 \) reduces to the one for standard TLS problem given in [20,23]. Moreover, the estimate in Theorem 3.4 becomes
\[
\Delta e = \kappa_{11s} \text{vec}(|\Delta A \quad \Delta b|) + O(||\Delta A \quad \Delta b||_F^2) \approx -(A^T A - \sigma_{n+1}^2 I_{n+1})^{-1} A^T H_0 (\Delta Ax - \Delta b) - (A^T A - \sigma_{n+1}^2 I_{n+1})^{-1} A^T H_r.
\]
By taking 2-norm of $\Delta x$, we obtain the relative perturbation result of the TLS solution as follows
\[
\frac{\|\Delta x\|_2}{\|x\|_2} \leq \kappa_b \frac{\|\Delta b\|_2}{\|b\|_2} + \kappa_A \frac{\|\Delta A\|_2}{\|A\|_2},
\] (4.3)
where $\kappa_b = \frac{\|b\|_2}{\|x\|_2} (A^T A - \sigma_n^2 I)^{-1} A^T \|x\|_2 \|b\|_2$ and
\[
\kappa_A = \frac{\|A\|_2}{\|x\|_2} \left( \left\| (A^T A - \sigma_n^2 I)^{-1} \right\|_2 + \|x\|_2 \right) (A^T A - \sigma_n^2 I)^{-1} A^T \|x\|_2 \|b\|_2.
\]
The perturbation estimate in (4.3) is the same as the result in [8].

For mixed and componentwise condition numbers, $\kappa_{L,h}$ in Theorem 5.5 reduces to
\[
\kappa_{L,h} = x^T \otimes [0_{n \times p} \ D] - P^{-1}(I_n \otimes [0_{1 \times p} \ r^T]) - [0_{n \times p} \ D],
\]
for $\tilde{D} = -P^{-1}(A^T - 2p^{-2}x r^T)$, and therefore $\kappa_m$ and $\kappa_c$ become
\[
\kappa_{L,h}^{\text{mix}} = \frac{||M||2 + |D||b|}{\|x\|_\infty}, \quad \kappa_{L,h}^{\text{comp}} = \frac{||M||2 + |D||b|}{\|x\|_\infty},
\]
where $M = (x^T \otimes \tilde{D}) - P^{-1}(I_n \otimes r^T)$. These results are exactly the ones from [8].

5 Numerical experiments

In this section, we present numerical examples to verify our results. The following numerical tests are performed via MATLAB with machine precision $u = 2.22 \times 10^{-16}$ in a laptop with Intel Core (TM) i5-5200U CPU. In all tests, we take $\alpha = \beta = 1$ in the normwise condition number $\kappa_n$ and its upper bound $\kappa_u$.

Example 5.1 In this example, we construct random TLSE problems in which the entries in the input matrices have equilibratory magnitude. Let $[A \ b]$ be a random matrix, and the matrix $\tilde{C} = [C \ d]$ be generated by
\[
\tilde{C} = Y[D \ 0] Z^T,
\]
where $Y = I_p - 2yy^T$, $Z = I_{n+1} - 2zz^T$, and $y \in \mathbb{R}^p, z \in \mathbb{R}^{n+1}$ are random unit vectors, $D$ is a $p \times p$ diagonal matrix whose diagonal entries are uniformly distributed in the interval $(0, 1)$ except the last one. The last diagonal entry is determined such that the condition number of $\tilde{C}$ is $\kappa_{\tilde{C}}$.

Consider random perturbations
\[
[\Delta L \ \Delta h] = 10^{-8} \times \text{rand}(p + q, n + 1),
\] (5.1)
and set
\[
\epsilon_1 = \frac{||\Delta L \ \Delta h||_F}{||[L \ b]||_F}, \quad \eta_{\Delta_L}^{\text{rel}} = \frac{||\Delta x - K_{L,h} \text{vec}([\Delta L \ \Delta h])||_2}{\|\Delta x\|_2},
\]
where $\eta_{\Delta_L}^{\text{rel}}$ is used to measure the correctness of Theorem 5.4 $\epsilon_1 \kappa_n$ with $\alpha = \beta = 1$ is used to estimate an upper bound of the relative forward error $\frac{||\Delta x||_2}{\|x\|_2}$.

In Table 5.1, we choose $p = 5, n = 15, q = 20$. For each given $\kappa_{\tilde{C}}$, we generate two different TLSE problems, and use the stable QR-SVD algorithm to compute the solutions to the original and perturbed problems. Relative forward error of the TLSE solution is compared with the estimated upper bounds via normwise condition numbers.

The tabulated results for $\eta_{\Delta_L}^{\text{rel}}$ show that the first order estimate for $\Delta x$ in Theorem 5.4 is reasonable. It is also observed that $(\epsilon_1 \kappa_n)$ is about one or two orders of magnitude larger than the actual relative forward error $\frac{||\Delta x||_2}{\|x\|_2}$, even the intermediate factor $||C_A||_2$ is large and the problem becomes ill-conditioned. The upper bound $\kappa_u$ is a tight estimate of the normwise condition number. This indicates that $\epsilon_1 \kappa_u$ can
be an alternative to estimate the forward error of the TLSE solution.

Example 5.2 In this example, we test the accuracy of the TLSE solution via the randomized algorithm in Algorithm 2.1, and also compare corresponding relative forward error of the solution with the estimated upper bounds for the perturbed TLSE problem. Let

\[
[L \ h] = Y \begin{bmatrix} A \\ 0 \end{bmatrix} Z^T \epsilon \subseteq \mathbb{R}^{(p+q)\times (n+1)}, \quad Y = I_{p+q} - 2yy^T, \quad Z = I_{n+1} - 2zz^T,
\]

where \(y \in \mathbb{R}^{p+q}, z \in \mathbb{R}^{(n+1)}\) are random unit vectors, \(A = \text{diag}(n, \ldots, 2, 1, \delta)\) with a positive parameter \(\delta\) close to 0.

Set \(m = 50\) or \(100\), \(p = 0.1m, n = 0.2m\), and denote

\[
E_{\text{nwtls}} = \frac{\|x_{\text{nwtls}} - x_{\text{qr-svd}}\|_2}{\|x_{\text{qr-svd}}\|_2},
\]

where \(x_{\text{nwtls}}, x_{\text{qr-svd}}\) are solutions of the unperturbed TLSE problem computed via NWTLS and QR-SVD methods, respectively, and for NWTLS method in Algorithm 2.1, we take the weighting factor \(\epsilon = 10^{-8}\) and the sample size \(\ell = 5\).

Generate random perturbation as in (5.1), and compute the solutions to the perturbed problem via NWTLS and QR-SVD algorithms, respectively. In Table 5.2, we list numerical results with respect to different parameters. It is observed that the randomized NWTLS algorithm can be as accurate as the QR-SVD method. One exception for \(E_{\text{nwtls}}\) is for \(\delta = 10^{-2}\), in which case the error \(E_{\text{nwtls}}\) is not close enough to machine precision. That is because when \(\delta = 10^{-2}\), the ratio between the subdominant and dominant eigenvalues of \((G^TG)^{-1}\) is not small enough to guarantee solutions with higher accuracy. We also note that the upper bounds \(\epsilon_1 \kappa_n, \epsilon_1 \kappa^U_n\) estimated via normwise condition number are sharp to evaluate the forward errors by the NWTLS algorithm.

Example 5.3 In this example, we do some numerical experiments for the TLSE problem, based on the piecewise-polynomial data fitting problem in [4, Chapter 16] and [7].

| \(\kappa_C\) | \(\|\tilde{C}\|_2\) | \(\eta_{\text{tlse}}^\dagger\) | \(\epsilon_1 \kappa_n\) | \(\epsilon_1 \kappa^U_n\) | \(\|C\|_2\) |
|---|---|---|---|---|---|
| 10 | 7.56e-7 | 1.29e-6 | 3.46e-5 | 2.12e-4 | 5.16e+2 |
| 10^2 | 2.90e-5 | 5.23e-5 | 5.63e-4 | 9.04e-3 | 2.61e+4 |
| 10^3 | 1.66e-5 | 8.11e-6 | 2.99e-5 | 8.11e-5 | 1.90e+2 |
| 10^4 | 9.93e-5 | 2.49e-4 | 2.12e-4 | 7.24e-4 | 5.37e+3 |
| 10^5 | 1.06e-3 | 5.23e-3 | 9.04e-3 | 1.90e+2 |

Example 5.3 In this example, we do some numerical experiments for the TLSE problem, based on the piecewise-polynomial data fitting problem in [4, Chapter 16] and [7].

| \(\delta\) | \(m\) | \(\text{cond}(AQ_2)\) | \(\epsilon_{1\kappa_n}\) | \(\epsilon_{1\kappa^U_n}\) |
|---|---|---|---|---|
| 1e-2 | 50 | 1.01e+3 | 4.21e-11 | 4.54e-7 |
| 1e-2 | 100 | 2.03e+3 | 7.84e-11 | 2.56e-6 |
| 1e-3 | 50 | 1.00e+4 | 4.90e-15 | 5.19e-7 |
| 1e-3 | 100 | 2.03e+4 | 1.25e-14 | 3.94e-6 |
| 1e-4 | 50 | 9.93e+4 | 1.45e-15 | 4.26e-7 |
| 1e-4 | 100 | 1.98e+5 | 3.09e-15 | 5.53e-7 |
Given \( N \) points \( (t_i, y_i) \) on the plane, we are seeking to find a piecewise-polynomial function \( f(t) \) fitting the above set of the points, where

\[
f(t) = \begin{cases} \ f_1(t), & t \leq a, \\ \ f_2(t), & t > a, \end{cases}
\]

with \( a \) given, and \( f_1(t) \) and \( f_2(t) \) polynomials of degree three or less,

\[
f_1(t) = x_1 + x_2 t + x_3 t^2 + x_4 t^3, \quad f_2(t) = x_5 + x_6 t + x_7 t^2 + x_8 t^3.
\]

The conditions that \( f_1(a) = f_2(a) \) and \( f_1'(a) = f_2'(a) \) are imposed, so that \( f(t) \) is continuous and has a continuous first derivative at \( t = a \). Suppose that the \( N \) data are numbered so that \( t_1, \ldots, t_M \leq a \) and \( t_{M+1}, \ldots, t_N > a \). The conditions \( f_1(a) - f_2(a) = 0 \) and \( f_1'(a) - f_2'(a) = 0 \) leads to the equality constraint \( Cx = d \) for \( x = [x_1 \ x_2 \ldots \ x_8]^T \) and

\[
C = \begin{bmatrix} 1 & a & a^2 & a^3 & -1 - a & -a^2 & -a^3 \\ 0 & 1 & 2a & 3a^2 & 0 & -1 - 2a & -3a^2 \end{bmatrix}, \quad d = \begin{bmatrix} 0 \\ 0 \end{bmatrix}.
\]

The vector \( x \) that minimizes the sum of squares of the prediction errors

\[
\sum_{i=1}^{M} (f_1(t_i) - y_i)^2 + \sum_{i=M+1}^{N} (f_2(t_i) - y_i)^2,
\]

gives \( \min_x \|Ax - b\|_2 \), where

\[
A = \begin{bmatrix} 1 & t_1 & t_1^2 & t_1^3 & 0 & 0 & 0 & 0 \\ 1 & t_2 & t_2^2 & t_2^3 & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & t_M & t_M^2 & t_M^3 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & t_{M+1} & t_{M+1}^2 & t_{M+1}^3 \\ 0 & 0 & 0 & 0 & 1 & t_{M+2} & t_{M+2}^2 & t_{M+2}^3 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 1 & t_N & t_N^2 & t_N^3 \end{bmatrix}, \quad b = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_M \\ y_{M+1} \\ \vdots \\ y_N \end{bmatrix},
\]

and the matrix \( A \) is of 50% sparsity. Take \( M = 200, N = 400 \), and let samples \( t_i \in [0, 1] \) randomly generated such that

\[
[t_1 \ldots \ t_M] = a \cdot E_{1,M}, \quad [t_{M+1} \ldots \ t_N] = a \cdot 1_{N-M}^T + (1 - a) \cdot E_{N-M},
\]

where \( E_{s,t} \) is a random \( s \times t \) matrix whose entries are uniformly distributed on the interval (0, 1), and \( 1_{N-M} \) is a column vector of all ones. For a randomly generated piecewise-polynomial function \( f(t) \) with a predetermined \( a \), we compute the corresponding function value \( y_i = f(t_i) \), and add random componentwise perturbations on the data as

\[
\Delta C = 10^{-8} \cdot E_{2,8} \odot C, \quad \Delta A = 10^{-8} \cdot E_{N,8} \odot A, \quad \Delta b = 10^{-8} \cdot E_{N,1} \odot b,
\]

and \( \Delta d = 0 \), where \( \odot \) denotes the entrywise multiplication. Set

\[
\epsilon_2 = \min \{ \epsilon : |\Delta L| \leq \epsilon |L|, |\Delta h| \leq \epsilon |h| \},
\]

then the relative errors \( \frac{\Delta x}{\|x\|_\infty}, \frac{\Delta x}{\|x\|_\infty} \) can be bounded by \( \epsilon_2 \kappa_m, \epsilon_2 \kappa_c \) respectively.

In Table 5.8 we list the actual forward errors and corresponding upper bounds estimated via different condition numbers. It’s observed that three types condition numbers multiplied by backward errors give good estimates of the forward error when \( a \geq 0.5 \), and they are about one or two orders of magnitude larger than the relative forward error, and the upper bounds of three types condition numbers are tight as well. The relative forward errors of the solution are almost about \( 10^{-7} \), except for the case \( a = 0.9 \). This
happens because in (2.15), the gap between the singular values $\sigma_{n-p} = 1.65e - 4$ and $\sigma_{n-p+1} = 1.62e - 4$ is very small, and the small gap not only makes the matrix $K$ to have large norm, but also leads to a small value $4.87e - 5$ in the last component of $Q_2\delta_{n-p+1}$, which also makes the solution $x$, vectors $r$ and $t$ in Theorem 5.4 to have large norms. These large values will magnify the backward errors and hence affect the magnitude of $\|\Delta x\|_2$.

On the other hand, we also note that when $a$ decreases, especially for $a = 0.05$, the forward error estimated via normwise condition number is far away from the true value of the forward error, while mixed and componentwise condition numbers and their upper bounds can still estimate the forward error very tightly. The reason is that when $a$ is small, $t_1, t_2, \ldots, t_N$ are of different magnitude, and $L$ is badly scaled, which causes different magnitude of entries in $K_{L,h}$. In the forward error estimated via normwise condition number, the condition number $\|K_{L,h}\|_2$ is dominated by its high-magnitude entries, while for mixed and componentwise condition number-based estimates, the high-magnitude entries in $|K_{L,h}|$ might be restrained by small or zero entries in $|L| \cdot |h|$, leading to tight estimates for the forward error of the solution.

| $a$   | $\frac{2\epsilon_1}{\|y\|}$ | $\epsilon_1^U$ | $\epsilon_2^U$ | $\epsilon_3^U$ | $\epsilon_4^U$ | $\epsilon_5^U$ | $\epsilon_6^U$ |
|-------|--------------------------|-------------|-------------|-------------|-------------|-------------|-------------|
| 0.05  | 1.87e-7                  | 5.69e-2     | 5.48e-1     | 1.87e-7     | 5.42e-6     | 6.41e-5     | 1.87e-7     | 9.01e-6     | 1.28e-4     |
| 0.1   | 3.46e-7                  | 9.60e-3     | 8.74e-2     | 3.46e-7     | 6.81e-6     | 7.34e-5     | 3.77e-7     | 9.42e-6     | 1.07e-4     |
| 0.3   | 2.04e-7                  | 1.28e-4     | 4.84e-4     | 2.05e-7     | 6.80e-6     | 2.00e-5     | 2.22e-7     | 8.09e-6     | 2.30e-5     |
| 0.5   | 4.24e-7                  | 5.42e-5     | 1.07e-4     | 4.36e-7     | 9.73e-6     | 2.04e-5     | 4.22e-7     | 1.04e-5     | 2.44e-5     |
| 0.7   | 1.76e-7                  | 2.56e-4     | 5.72e-4     | 1.67e-7     | 5.96e-5     | 1.33e-4     | 2.58e-7     | 6.10e-5     | 1.36e-4     |
| 0.9   | 5.25e-4                  | 2.45e-2     | 1.43e-1     | 5.25e-4     | 3.30e-3     | 7.82e-2     | 1.18e-3     | 7.83e-3     | 2.96e-1     |

6 Conclusion and future work

In this paper, by making use of a limit technique, we present the closed formula for the first order perturbation estimate of the TLSE solution, based on which normwise, mixed and componentwise condition numbers of problem TLSE are derived. Since these expressions all involve matrix Kronecker product operations, we propose different skills to simplify the expressions to improve the computational efficiency. For the normwise condition number, the alternative expression and upper bound in Theorem 4.2 is more compact and shown to be tight for TLSE problems with equilibratory input data. The computation of $\kappa_n$, the main cost involves formulating $H_1, K$, computing an $n \times (n + m)$ matrix and evaluating its 2-norm as well.

For mixed and componentwise condition numbers, the Kronecker product operation in $K_{L,h}$ also increase the storage and computational cost. According to the numerical experiments, the upper bounds are very sharp and can be suitable to measure the conditioning of the TLSE problem, especially for sparse and badly-scaled TLSE problems. In the computation of the upper bounds, the main cost is the formulation of matrices $H_1, K$, the remaining cost involves the cheap matrix-vector multiplications and the infinity-norm evaluation of the vectors, therefore the computation and storage is more economical than the one for normwise condition number.

In the future work, we are going to investigate the perturbation result of the TLSE problem, in which the different magnitudes of perturbations in input data are taken into account. The proposed results are expected to deliver better estimates of forward errors of the solution than the one based on normwise condition number. The condition number of the following multidimensional TLSE problem

$$\min_{E,F} \|[E \quad F]\|_2, \text{ subject to } (A + E)X = B + F, \quad CX = D,$$

are also considered, where $A, E \in \mathbb{R}^{q \times n}$, $B, F \in \mathbb{R}^{q \times d}$, $C \in \mathbb{R}^{p \times n}$, $D \in \mathbb{R}^{p \times d}$.
When $C, D$ are zero matrices, the problem reduces to the multidimensional TLS problem, whose condition numbers have been investigated in [31, 52]. It is of interest to make use of the similar limit technique to investigate the condition numbers of the multidimensional TLSE problem. However, the discussions on solvability conditions and the explicit solution to the multidimensional TLSE problem haven’t been seen in the literature. Compared to condition numbers of the (single-right-hand) TLSE problem [11], the multidimensional case is more complicated since the smallest singular value of $\tilde{A}Q_2$ might be multiple and the corresponding singular vector is not unique and lies in an invariant subspace. This brings difficulty in establishing the close relation between multidimensional TLSE and multidimensional WTLS problems. Moreover those techniques in [27] can not be used. New tools are needed in dealing with the subspace approximation problem. We will investigate these issues in a separate paper [26].

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