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Perturbation analysis for mixed least squares–total least squares problems

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Summary

In many linear parameter estimation problems, one can use the mixed least squares–total least squares (MTLS) approach to solve them. This paper is devoted to the perturbation analysis of the MTLS problem. Firstly, we present the normwise, mixed, and componentwise condition numbers of the MTLS problem, and find that the normwise, mixed, and componentwise condition numbers of the TLS problem and the LS problem are unified in the ones of the MTLS problem. In the analysis of the first-order perturbation, we first provide an upper bound based on the normwise condition number. In order to overcome the problems encountered in calculating the normwise condition number, we give an upper bound for computing more effectively for the MTLS problem. As two estimation techniques for solving the linear parameter estimation problems, interesting connections between their solutions, their residuals for the MTLS problem, and the LS problem are compared. Finally, some numerical experiments are performed to illustrate our results.

KEYWORDS

condition number, mixed least squares–total least squares, perturbation analysis, perturbation bound, weighted total least squares

1 | INTRODUCTION

Many problems in data fitting and estimation come down to solving an overdetermined system of linear equations $Ax \approx b$, where $A \in \mathbb{R}^{m\times n}(m \geq n)$ and $b \in R^m$. In the classical least squares (LS) approach, the input data matrix A are assumed to be free of error, and hence, all errors are confined to the observation vector b. However, this assumption is frequently unrealistic because sampling errors, human errors, modeling errors, and instrument errors may imply inaccuracies of the data matrix A, that is, both the data matrix A and the observation vector b are contaminated by noise. In this case, the total least squares (TLS) approach has been devised and amounts to fitting the "best" subspace to the measurement data $[A, b]$, that is, to seek a perturbation matrix $E \in \mathbb{R}^{m\times n}$ and a perturbation vector $f \in \mathbb{R}^m$ that minimize $\|[E, f]\|_F$ subject to the consistency equation $(A + E)x = b + f$, where $\|\cdot\|_F$ denotes the Frobenius norm of a matrix. The TLS approach has been widely used in a variety of scientific disciplines, and therefore, its properties were deeply studied in the works of Golub et al.[1] and Van Huffel et al.,[2,3] and the references therein.

However, in many linear parameter estimation problems, some entries of the data matrix A on the left side of the approximate system $Ax \approx b$ may be observed without error. For instance, in regression analysis,[4] system identification,[5] and signal processing,[6] some signals can be observed without error, whereas the other ones are disturbed by zero-mean white noise. Another typical example is the problem of the space (e.g., GPS) coordinate transformation using the Bursa model,[7] where the translation parameters are usually considered accurate. These problems often result in the case that some of the columns of data matrix A are exact. Hence, to maximize the accuracy of the estimated parameters x, the case that some of the columns in data matrix A are error free whereas others are perturbed is naturally considered when estimating parameter x using the TLS approach. The TLS problem with some exact columns in the data matrix was known as a mixed errors-in-variables (MEIV) model in the statistics literature,[3] the general errors-in-variables model in the work of Van Huffel et al.,[8] the mixed LS-TLS method in the work of Golub et al.,[9] or the mixed least squares–total least squares (MTLS) problem in the works of Liu et al.[10] and Yan et al.[11] For the convenience of the later discussion, from now on, we call it the MTLS problem as a unified name. Obviously, the MTLS problem is a generalization of the classic TLS problem and the LS problem.

In 1987, Golub et al.[9] developed a standard QR-SVD algorithm for solving the MTLS problem through factorizing the augmented matrix $[A, b]$ into a QR form first and then solving a reduced TLS problem using singular value decomposition (SVD). Later, Van Huffel et al.[8] extended The MTLS problem with a single right-hand side to the multiple right-hand case and provided a computationally efficient and numerically reliable algorithm based on the generalized SVD (GSVD). Recently, Liu et al.[10] have interpreted the MTLS solution as a limit of the solution to a weighted TLS problem, as the positive parameter in the weight matrix tends to zero, and presented a Cholesky factorization-based inverse (Cho-INV) iteration and a Rayleigh quotient iteration method. The superiority of their methods over the standard QR-SVD algorithm was demonstrated by numerical experiments. However, as far as we know, the perturbation analysis of the MTLS problem has not been systematically performed in the literature. Hence, in this paper, we are concerned with this topic and the main tools used are the weighted method presented in the work of Liu et al.[10] and the SVD of a matrix.

This paper is organized as follows. In Section 2, we briefly review the QR-SVD algorithm and the weighted TLS method for solving the MTLS problem. Because condition numbers often measure the sensitivity of the solution to the original data in problems and therefore play an important role in numerical analysis, the closed forms of the normwise, mixed, and componentwise condition numbers of the solution to MTLS problem are derived via the associated weighted TLS method in Section 3. Section 4 mainly gives an upper-bound estimate of the relative error of the MTLS solution based on the normwise condition number and a more effective upper-bound estimate, which can overcome the problems encountered in calculating the normwise condition number. Numerical examples show that our bounds are superior to that of Wei et al.[12] Section 5 compares the MTLS solution with the LS solution and provides the lower and upper bounds of the difference among these two kind of solutions, as well as their corresponding residuals. Some numerical experiments are given to demonstrate our theoretical results in Section 6, and then, we conclude the paper in Section 7.

Throughout this paper, we denote by $\mathbb{R}^{m\times n}$ the space of all $m \times n$ real matrices; $\mathbb{R}^m$ denotes the space of m-dimensional real column vectors. $\|\cdot\|_2$, $\|\cdot\|_\infty$ and $\|\cdot\|_F$ denote the 2-norm, ∞-norm, and Frobenius norm of their arguments, respectively. Given a matrix $X = [x_{ij}] \in \mathbb{R}^{m\times n}$, X^T and $\sigma_i(X)$ denote the transpose and the ith largest singular value of X, respectively. Single vertical bars around a matrix or vector indicate the componentwise absolute value of a matrix or vector. As usual, I_n denotes the identity matrix of order n and $\mathbf{0}_{m,n}$ is the $m \times n$ matrix with all zero entries (if no confusion occurs, we drop the subscript). In addition, let $P \in \mathbb{R}^{mn\times mn}$ denote the permutation matrix that represents the matrix transpose by $\mathrm{vec}(B^T) = P\mathrm{vec}(B)$. For $A = (a_1, \ldots, a_n) \in \mathbb{R}^{m\times n}$, $\mathrm{vec}(A) = (a_1^T, \ldots, a_n^T)^T \in \mathbb{R}^{mn\times 1}$.

2 | THE QR-SVD ALGORITHM AND THE WEIGHTED METHOD

For the overdetermined linear system, $Ax \approx b$, where $A = (A_1, A_2)$ with $A_1 \in R^{m\times n_1}$, $A_2 \in R^{m\times n_2}$, and $n_1 + n_2 = n$. Assume the columns of A_1 are known exactly and A is of full column rank. If we partition the vector x as $x = (x_1, x_2)^T$ with $x_1 \in R^{n_1}$ and $x_2 \in R^{n_2}$, then the following optimization problem is called the MTLS problem:

$$\min_{E_2, f} \|(E_2, f)\|_F, \quad \text{s.t.} \quad A_1x_1 + (A_2 + E_2)x_2 = b + f. \tag{1}$$

Obviously, if $n_1 = 0$, the MTLS problem will become a TLS problem, whereas if $n_2 = 0$, it will reduce to an LS problem. To solve MTLS problem (1), we first factorize (A, b) into the QR form

$$Q^T(A_1, A_2, b) = R = \begin{array}{cc} \begin{array}{ccc} n_1 & n_2 & 1 \end{array} & \\ \begin{bmatrix} R_{11} & R_{12} & R_{1b} \\ 0 & R_{22} & R_{2b} \end{bmatrix} & \begin{array}{c} n_1 \\ m - n_1 \end{array} \end{array}, \tag{2}$$

and then solve the reduced TLS problem for the approximate linear system $R_{22}x_2 \approx R_{2b}$, which can be solved by the standard SVD approach. The vector x_1 can be obtained from $R_{11}x_1 = R_{1b} - R_{12}x_2$ by back substitution. Let $\sigma_j(A)$ denote the jth largest singular value of A. We know that, under the condition

$$\sigma = \sigma_{n_2}(R_{22}) > \tilde{\sigma} = \sigma_{n_2+1}(R_{22}, R_{2b}) > 0, \tag{3}$$

the reduced TLS problem and, therefore, the MTLS have a unique solution[8]:

$$x_{\mathrm{MTLS}} = (A^T A - \tilde{\sigma}^2 C)^{-1} A^T b, \quad C = \begin{pmatrix} 0 & 0 \\ 0 & I_{n_2} \end{pmatrix}. \tag{4}$$

The abovementioned approach for solving the MTLS problem (1) is called the standard QR-SVD algorithm.[9] Recently, a weighted method has been described in the work of Liu et al.[10] It is proved that the MTLS problem can be regarded as the limit case of the WTLS problem

$$\min_{E,f} \|(E, f)\|_F, \quad \text{s.t.} \quad (A_\varepsilon + E) C_\varepsilon x_\varepsilon = b + f, \tag{5}$$

when ε tends to 0, where $A_\varepsilon = AC_\varepsilon^{-1}$ with $C_\varepsilon = \begin{pmatrix} \varepsilon I_{n_1} & 0 \\ 0 & I_{n_2} \end{pmatrix}$ and ε is a small positive number. Under the assumption of genericity condition (3) and the assumption

$$\varepsilon^2 \left\|A_1^\dagger\right\|_2^2 \|\tilde{A}_2\|_2^2 < \frac{\sigma^2 - \tilde{\sigma}^2}{2\sigma^2}, \tag{6}$$

the WTLS solution x_ε is unique and can be represented as

$$x_\varepsilon = C_\varepsilon^{-1} \left(A_\varepsilon^T A_\varepsilon - \bar{\sigma}_{n+1}^2 I\right)^{-1} A_\varepsilon^T b \tag{7}$$

and

$$x_{\mathrm{MTLS}} = \lim_{\varepsilon \to 0^+} x_\varepsilon, \tag{8}$$

where $\bar{\sigma}_{n+1}$ is the smallest singular value of (A_ε, b) and $\tilde{A}_2 = (A_2, b)$. Throughout this paper, we assume that the conditions (3) and (6) hold.

In this paper, the perturbation analysis of the MTLS problem is deduced by means of its weighting method, and the calculation of the results still needs the QR-SVD algorithm.

3 | CONDITION NUMBERS OF THE MTLS PROBLEM

In this section, we will derive the exact formula of the normwise, mixed, and componentwise condition numbers of the solution to the MTLS problem (1).

As we know, when formulating the MTLS problem, one assumes that the matrix A_1 is known exactly, and therefore, so are its structure and rank. We are then interested in how perturbations in A_2 and b effect the solution. In the practical computation of the MTLS solution, one can apply the standard QR-SVD algorithm mentioned above. However, because of finite precision computation, even using a numerically stable algorithm in the computation will produce computed errors corresponding to slightly different initial data. Notice that, in general, this effective error in the initial matrices due to round off is much smaller than the error caused by uncertainty in the data. To simplify the analysis, we therefore make the following assumptions, which allow any perturbations in A_2 and b, but only relatively small perturbations in A_1. This means that we can assume $\tilde{A} = A + \Delta A$ and $\tilde{b} = b + \Delta b$, where $\Delta A = [\Delta A_1, \Delta A_2]$ and Δb are the perturbations of the input data A and b, respectively. As for ΔA, we have that ΔA_1 is much smaller than ΔA_2. We let $\widetilde{x}_{\mathrm{MTLS}}$ be the MTLS solution to the perturbed approximate system $\widetilde{A}x \approx \widetilde{b}$ or the perturbed MTLS problem associated with the matrices $\widetilde{A}$ and $\widetilde{b}$. If the norm $\|[\Delta A, \Delta b]\|_F$ of the perturbations is sufficiently small, then perturbation analysis for the QR factorization[13] and perturbation analysis of singular values ensure that the perturbed MTLS problem above has a unique solution $\widetilde{x}_{\mathrm{MTLS}}$.

Because condition numbers often measure the sensitivity of the solution to the original data in problems, they play an important role in numerical analysis. In addition, if the MTLS solution is a differentiable function with respect to the data, then the condition numbers can be exactly expressed in derivatives. Unfortunately, there is certain difficulty to derive the condition numbers of x_{MTLS} directly via this approach to the MTLS problem. Therefore, we start from the differentiability of the weighted TLS solution x_ε and the MTLS solution x_{MTLS} and, then, take the limits as the parameter ε approaches zero to get the various condition numbers of the MTLS solution x_{MTLS}.

Let $\tilde{A}_\varepsilon = A_\varepsilon + \Delta A_\varepsilon$ and $\tilde{b} = b + \Delta b$, where ΔA_ε and Δb are the perturbations of the input data A_ε and b, respectively. Consider the perturbed WTLS problem $\min_{E,f} \|[E, f]\|_F$ s.t. $(\tilde{A}_\varepsilon + E) C_\varepsilon \tilde{x}_\varepsilon = \tilde{b} + f$. If the norm $\|(\Delta A_\varepsilon, \Delta b)\|_F$ of the perturbations is sufficiently small, then the well-known perturbation analysis of singular values ensures that the perturbed WTLS problem above has a unique solution $\tilde{x}_\varepsilon$, which can be expressed as same as that in (7). The two perturbation matrices $[\Delta A, \Delta b]$ and $[\Delta A_\varepsilon, \Delta b]$ should be small enough to ensure the existence and uniqueness of the perturbation MTLS solution and the perturbation WTLS solution, simultaneously. Under the assumption $\Delta A_\varepsilon = \Delta A C_\varepsilon^{-1}$, we can achieve the effect that the perturbation of A_1 is much smaller than that of A_2 for the MTLS problem and have $\widetilde{x}_{\mathrm{MTLS}} = \lim_{\varepsilon\to 0^+}\tilde{x}_\varepsilon$, which coincides with our expectation about the perturbations of the input data A and b and is worth celebrating. We attribute the success to the works of Liu et al.[10] and Wei et al.[12]

To derive the exact formulae of the condition numbers of x_{MTLS}, we define the mapping $\varphi([A,b]) : \mathbb{R}^{m\times n}\times\mathbb{R}^m \to \mathbb{R}^n : [A,b] \mapsto x_{\mathrm{MTLS}}$. The condition number of a mapping measures the sensitivity of the output to perturbations in input data. The Fréchet derivative is the linear operator $\varphi'([A,b])$ uniquely defined by the relation

$$\varphi\left([A,b]+[\Delta A,\Delta b]\right) = \varphi([A,b]) + \varphi'([A,b])\cdot[\Delta A,\Delta b] + \mathcal{O}(\|[\Delta A,\Delta b]\|), \tag{9}$$

whereas the (absolute) condition number of $\varphi([A,b])$ is defined as

$$\kappa^{\mathrm{abs}}(x_{\mathrm{MTLS}},A,b) = \lim_{\eta\to 0}\sup_{\|[\Delta A,\Delta b]\|_F\le\eta}\frac{\|\varphi([A,b]+[\Delta A,\Delta b])-\varphi([A,b])\|_2}{\|[\Delta A,\Delta b]\|_F}.$$

We know that, under assumption (3), x_2 is Fréchet differentiable in a neighborhood of $[A,b]$. For x_1, it can be obtained from $R_{11}x_1 = R_{1b} - R_{12}x_2$. Combined with the above two aspects, we can see that $\varphi([A,b])$ is Fréchet differentiable in a neighborhood of $[A,b]$.

Similarly, we can have the mapping for the WTLS problem

$$\phi([A_\varepsilon,b]+[\Delta A_\varepsilon,\Delta b]) = \phi([A_\varepsilon,b])+\phi'([A_\varepsilon,b])\cdot[\Delta A_\varepsilon,\Delta b] + \mathcal{O}(\|[\Delta A_\varepsilon,\Delta b]\|). \tag{10}$$

It is easy to know that $\phi([A_\varepsilon,b])$ is also Fréchet differentiable in a neighborhood of $[A_\varepsilon,b]$. Thus, there would be

$$\lim_{\varepsilon\to 0^+}\phi'([A_\varepsilon,b])\cdot[\Delta A_\varepsilon,\Delta b] = \varphi'([A,b])\cdot[\Delta A,\Delta b] \tag{11}$$

and one can get the expression for $\varphi'([A,b])$; see details in Lemma 1. Furthermore, following the work of Geurts,[14] if φ is Fréchet differentiable in a neighborhood of $[A,b]$, we have

$$\kappa^{\mathrm{abs}}(x_{\mathrm{MTLS}},A,b) = \|\varphi'([A,b])\|_2,\quad \kappa^{\mathrm{rel}}(x_{\mathrm{MTLS}},A,b) = \frac{\|\varphi'([A,b])\|_2\|[A,b]\|_F}{\|x_{\mathrm{MTLS}}\|_2}, \tag{12}$$

$$\kappa^{\mathrm{mix}}(x_{\mathrm{MTLS}},A,b) = \frac{\||\varphi'([A,b])|\mathrm{vec}([|A|,|b|])|\|_\infty}{\|x_{\mathrm{MTLS}}\|_\infty},\quad \kappa^{\mathrm{com}}(x_{\mathrm{MTLS}},A,b) = \left\|\frac{|\varphi'([A,b])|\mathrm{vec}([|A|,|b|])}{x_{\mathrm{MTLS}}}\right\|_\infty. \tag{13}$$

The next lemma proves that $\varphi([A,b])$ is Fréchet differentiable in a neighborhood of $[A,b]$ and gives the explicit expression for $\varphi'([A,b])$ after getting the Fréchet derivative for the WTLS problem and using (11). Therefore, we can easily get the formulae for the normwise, mixed, and componentwise condition numbers of x_{MTLS} by using (12), (13), and Lemma 1. In the rest of this paper, we may denote $x = x_{\mathrm{MTLS}}$ for simplicity.

Lemma 1. *Under genericity assumption (3), $\varphi([A,b])$ is Fréchet differentiable in a neighborhood of $[A,b]$. Then, the Fréchet derivative of $\varphi([A,b])$ at $[A,b]$ is expressed by*

$$\varphi'([A,b]) = H(A,b) = \left(-[x^T\otimes D] + [r^T\otimes B^{-1}]P, D\right), \tag{14}$$

where $B = A^TA - \tilde{\sigma}^2C$, $D = B^{-1}(A^T + 2\frac{Cxr^T}{\bar{\gamma}})$, $\bar{\gamma} = 1+\|Cx\|_2^2$, x is the exact solution of the MTLS problem (1), and r is the MTLS residual.

Proof. Equation (11) tells us that we just need to do the following two steps to prove the result.

1. The Fréchet derivative of $\phi([A_\varepsilon,b])$ at $[A_\varepsilon,b]$ is obtained from the chain rule. Let $\bar{\lambda}_{n+1} \equiv \bar{\sigma}_{n+1}^2$ be the smallest simple eigenvalue of $(A_\varepsilon,b)^T(A_\varepsilon,b)$ with corresponding unit eigenvector $\frac{1}{\sqrt{1+\|C_\varepsilon x_\varepsilon\|_2^2}}\begin{pmatrix}C_\varepsilon x_\varepsilon\\-1\end{pmatrix}$ and $\gamma_\varepsilon = 1+\|C_\varepsilon x_\varepsilon\|_2^2$.

We know $\bar{\lambda}_{n+1}$ is differentiable in a neighborhood of (A_ε, b), and then, we have

$$\begin{aligned}
\bar{\lambda}'_{n+1}([A_\varepsilon, b]).[\Delta A_\varepsilon, \Delta b] &= \frac{1}{\gamma_\varepsilon}\begin{pmatrix}(C_\varepsilon x_\varepsilon)^T & -1\end{pmatrix}\begin{pmatrix}\Delta A_\varepsilon^T A_\varepsilon + A_\varepsilon^T \Delta A_\varepsilon & \Delta A_\varepsilon^T b + A_\varepsilon^T \Delta b \\ b^T \Delta A_\varepsilon + \Delta b^T A_\varepsilon & \Delta b^T b + b^T \Delta b\end{pmatrix}\begin{pmatrix}C_\varepsilon x_\varepsilon \\ -1\end{pmatrix} \\
&= \frac{2}{\gamma_\varepsilon}\left((C_\varepsilon x_\varepsilon)^T \Delta A_\varepsilon^T A_\varepsilon C_\varepsilon x_\varepsilon - (C_\varepsilon x_\varepsilon)^T \Delta A_\varepsilon^T b - (C_\varepsilon x_\varepsilon)^T A_\varepsilon^T \Delta b + b^T \Delta b\right) \\
&= \frac{2}{\gamma_\varepsilon}\left(-(C_\varepsilon x_\varepsilon)^T \Delta A_\varepsilon^T r_\varepsilon + \left(b^T - (C_\varepsilon x_\varepsilon)^T A_\varepsilon^T\right)\Delta b\right) \\
&= \frac{2 r_\varepsilon^T (\Delta b - \Delta A_\varepsilon C_\varepsilon x_\varepsilon)}{\gamma_\varepsilon}.
\end{aligned}$$

Applying the chain rule to $B_\varepsilon \equiv (A_\varepsilon^T A_\varepsilon - \bar{\sigma}_{n+1}^2 I)^{-1}$, we obtain

$$\begin{aligned}
B'_\varepsilon([A_\varepsilon, b]).([\Delta A_\varepsilon, \Delta b]) &= -B_\varepsilon^{-1}\left(\Delta A_\varepsilon^T A_\varepsilon + A_\varepsilon^T \Delta A_\varepsilon - \bar{\lambda}'_{n+1}([A_\varepsilon, b]).[\Delta A_\varepsilon, \Delta b] I\right) B_\varepsilon^{-1} \\
&= -B_\varepsilon^{-1}\left(\Delta A_\varepsilon^T A_\varepsilon + A_\varepsilon^T \Delta A_\varepsilon - \frac{2 r_\varepsilon^T (\Delta b - \Delta A_\varepsilon C_\varepsilon x_\varepsilon)}{\gamma_\varepsilon} I\right) B_\varepsilon^{-1}.
\end{aligned}$$

The chain rule now applied to $\phi([A_\varepsilon, b])$ leads to

$$\phi'([A_\varepsilon, b]).[\Delta A_\varepsilon, \Delta b] = C_\varepsilon^{-1} B_\varepsilon^{-1}\left(A_\varepsilon^T + 2\frac{C_\varepsilon x_\varepsilon r_\varepsilon^T}{\gamma_\varepsilon}\right)(\Delta b - \Delta A_\varepsilon C_\varepsilon x_\varepsilon) + C_\varepsilon^{-1} B_\varepsilon^{-1} \Delta A_\varepsilon^T r_\varepsilon.$$

We know $\phi'([A_\varepsilon, b]).[\Delta A_\varepsilon, \Delta b] = \mathrm{vec}(\phi'([A_\varepsilon, b]).[\Delta A_\varepsilon, \Delta b])$; if setting $D_\varepsilon = B_\varepsilon^{-1}(A_\varepsilon^T + 2\frac{C_\varepsilon x_\varepsilon r_\varepsilon^T}{\gamma_\varepsilon})$, then we have

$$\phi'([A_\varepsilon, b]).[\Delta A_\varepsilon, \Delta b] = \left(-\left[(C_\varepsilon x_\varepsilon)^T \otimes \left(C_\varepsilon^{-1} D_\varepsilon\right)\right] + \left[r_\varepsilon^T \otimes \left(C_\varepsilon^{-1} B_\varepsilon^{-1}\right)\right] P, C_\varepsilon^{-1} D_\varepsilon\right)\begin{pmatrix}\mathrm{vec}(\Delta A_\varepsilon) \\ \Delta b\end{pmatrix} \tag{15}$$

and we now obtain the matrix $M_{\phi'}$ representing $\phi'([A_\varepsilon, b])$, that is, such that

$$\begin{aligned}
\phi'([A_\varepsilon, b]).[\Delta A_\varepsilon, \Delta b] &= \left(-\left[(C_\varepsilon x_\varepsilon)^T \otimes \left(C_\varepsilon^{-1} D_\varepsilon\right)\right] + \left[r_\varepsilon^T \otimes \left(C_\varepsilon^{-1} B_\varepsilon^{-1}\right)\right] P, C_\varepsilon^{-1} D_\varepsilon\right)\begin{pmatrix}\mathrm{vec}(\Delta A_\varepsilon) \\ \Delta b\end{pmatrix} \\
&= M_{\phi'}\begin{pmatrix}\mathrm{vec}(\Delta A_\varepsilon) \\ \Delta b\end{pmatrix}.
\end{aligned}$$

2. Now, we can get the Fréchet derivative of $\varphi([A, b])$ at $[A, b]$ by the relationship between differentiability and derivability of $\varphi([A, b])$ and $\phi([A_\varepsilon, b])$, and (8). By (15), we have

$$\begin{aligned}
\varphi'([A, b]).[\Delta A, \Delta b] &= \mathrm{vec}\left(D(\Delta b - \Delta A x) + B^{-1} \Delta A^T r\right) \\
&= \left(-[x^T \otimes D] + [r^T \otimes B^{-1}] P, D\right)\begin{pmatrix}\mathrm{vec}(\Delta A) \\ \Delta b\end{pmatrix},
\end{aligned} \tag{16}$$

where $B = A^T A - \tilde{\sigma}^2 C$ and $D = B^{-1}(A^T + 2\frac{C x r^T}{\tilde{\gamma}})$. Let $H(A, b) = (-[x^T \otimes D] + [r^T \otimes B^{-1}] P, D)$; then, the result happens. □

3.1 | Normwise condition number

In this subsection, we present the closed formulas for the absolute and relative normwise condition numbers of x, which are first given in the following theorem.

Theorem 1. *Let $H(A, b)$ be defined as in Lemma 1 and assume that genericity assumption (3) holds. Then, the condition number of x of the MTLS solution is given by*

$$\kappa^{\mathrm{abs}}(x_{\mathrm{MTLS}}, A, b) = \|H(A, b)\|_2^{\frac{1}{2}}, \quad \kappa^{\mathrm{rel}}(x_{\mathrm{MTLS}}, A, b) = \|H(A, b)\|_2^{1/2} \frac{\|[A, b]\|_F}{\|x\|_2}. \tag{17}$$

Proof. The proof is easy to obtain by Lemma 1 and (12), and we omit it here. □

For large values of n or m, it is difficult, or even impossible, to build explicitly the generally dense matrix $H(A, b)$. Therefore, it is necessary to do further simplification. Before it, we remind the reader that $\mathrm{vec}(AXB) = (B^T \otimes A)\mathrm{vec}(X)$, where $\otimes$ denotes the Kronecker product of two matrices.[15]

Theorem 2. *Set $B = A^TA - \tilde{\sigma}^2 C$ and assume that genericity assumption (3) holds. Then, the condition number of x of the MTLS solution is expressed by*

$$\kappa^{\mathrm{abs}}(x_{\mathrm{MTLS}}, A, b) = \|M\|_2^{\frac{1}{2}}, \quad \kappa^{\mathrm{rel}}(x_{\mathrm{MTLS}}, A, b) = \|M\|_2^{1/2} \frac{\|[A, b]\|_F}{\|x\|_2}, \tag{18}$$

where M is the $n \times n$ matrix

$$M = \gamma B^{-1} \left(A^TA + \tilde{\sigma}^2 \bar{\gamma} \left(I - 2\frac{Cxx^TC}{\bar{\gamma}} \right) \right) B^{-1}, \tag{19}$$

$\bar{\gamma} = 1 + \|Cx\|_2^2$, $\gamma = 1 + \|x\|_2^2$, x is the exact solution of the MTLS problem, and r is the MTLS residual.

Proof. We find it difficult to simplify $H(A, b)$ directly. Therefore, we rely on $M_{\phi'}$ and have $(\kappa^{\mathrm{abs}}(x_\varepsilon, A_\varepsilon, b))^2 = \|M_{\phi'}^T\|_2^2 = \max_{\|y\|_2=1} \|M_{\phi'}^T y\|_2^2$. If y is a unit vector in R^n, then

$$\begin{aligned}
M_{\phi'}^T y &= \begin{pmatrix} -(C_\varepsilon x_\varepsilon) \otimes \left(C_\varepsilon^{-1} D_\varepsilon\right)^T + P^T r_\varepsilon \otimes \left(C_\varepsilon^{-1} B_\varepsilon^{-1}\right)^T \\ \left(C_\varepsilon^{-1} D_\varepsilon\right)^T \end{pmatrix} y \\
&= \begin{pmatrix} -(C_\varepsilon x_\varepsilon) \otimes \left(C_\varepsilon^{-1} D_\varepsilon\right)^T \mathrm{vec} y + P^T r_\varepsilon \otimes \left(C_\varepsilon^{-1} B_\varepsilon^{-1}\right)^T \mathrm{vec} y \\ \left(C_\varepsilon^{-1} D_\varepsilon\right)^T y \end{pmatrix} \\
&= \begin{pmatrix} P^{-1} \mathrm{vec} \left(-C_\varepsilon x_\varepsilon y^T C_\varepsilon^{-1} D_\varepsilon + \left(C_\varepsilon^{-1} B_\varepsilon^{-1}\right)^T y r_\varepsilon^T \right) \\ \left(C_\varepsilon^{-1} D_\varepsilon\right)^T y \end{pmatrix} \\
&= \begin{pmatrix} \mathrm{vec} \left(-(C_\varepsilon^{-1} D_\varepsilon)^T y (C_\varepsilon x_\varepsilon)^T + r_\varepsilon y^T C_\varepsilon^{-1} B_\varepsilon^{-1} \right) \\ \left(C_\varepsilon^{-1} D_\varepsilon\right)^T y \end{pmatrix}.
\end{aligned} \tag{20}$$

Then, we obtain

$$\begin{aligned}
\|M_{\phi'}^T y\|_2^2 &= \left\| \mathrm{vec} \left(-\left(C_\varepsilon^{-1} D_\varepsilon\right)^T y (C_\varepsilon x_\varepsilon)^T + r_\varepsilon y^T C_\varepsilon^{-1} B_\varepsilon^{-1} \right) \right\|_2^2 + \left\| \left(C_\varepsilon^{-1} D_\varepsilon\right)^T y \right\|_2^2 \\
&= \left\| -\left(C_\varepsilon^{-1} D_\varepsilon\right)^T y (C_\varepsilon x_\varepsilon)^T + r_\varepsilon y^T C_\varepsilon^{-1} B_\varepsilon^{-1} \right\|_F^2 + \left\| \left(C_\varepsilon^{-1} D_\varepsilon\right)^T y \right\|_2^2 \\
&= \left\| \left(C_\varepsilon^{-1} D_\varepsilon\right)^T y (C_\varepsilon x_\varepsilon)^T \right\|_F^2 + \|r_\varepsilon y^T C_\varepsilon^{-1} B_\varepsilon^{-1}\|_F^2 \\
&\quad - 2\mathrm{tr} \left(C_\varepsilon x_\varepsilon y^T C_\varepsilon^{-1} D_\varepsilon r_\varepsilon y^T C_\varepsilon^{-1} B_\varepsilon^{-1} \right) + \left\| \left(C_\varepsilon^{-1} D_\varepsilon\right)^T y \right\|_2^2 \\
&= \|C_\varepsilon x_\varepsilon\|_2^2 \left\| \left(C_\varepsilon^{-1} D_\varepsilon\right)^T y \right\|_2^2 + \|r_\varepsilon\|_2^2 \left\| \left(C_\varepsilon^{-1} B_\varepsilon^{-1}\right)^T y \right\|_2^2 \\
&\quad - 2y^T C_\varepsilon^{-1} B_\varepsilon^{-1} C_\varepsilon x_\varepsilon r_\varepsilon^T \left(C_\varepsilon^{-1} D_\varepsilon\right)^T y + \left\| \left(C_\varepsilon^{-1} D_\varepsilon\right)^T y \right\|_2^2 \\
&= \left(1 + \|C_\varepsilon x_\varepsilon\|_2^2\right) y^T C_\varepsilon^{-1} D_\varepsilon \left(C_\varepsilon^{-1} D_\varepsilon\right)^T y + \|r_\varepsilon\|_2^2 y^T C_\varepsilon^{-1} B_\varepsilon^{-1} \left(C_\varepsilon^{-1} B_\varepsilon^{-1}\right)^T y \\
&\quad - 2y^T C_\varepsilon^{-1} B_\varepsilon^{-1} C_\varepsilon x_\varepsilon r_\varepsilon^T \left(C_\varepsilon^{-1} D_\varepsilon\right)^T y \\
&= y^T \left(\gamma_\varepsilon C_\varepsilon^{-1} D_\varepsilon \left(C_\varepsilon^{-1} D_\varepsilon\right)^T + \|r_\varepsilon\|_2^2 C_\varepsilon^{-1} B_\varepsilon^{-1} \left(C_\varepsilon^{-1} B_\varepsilon^{-1}\right)^T \right. \\
&\quad \left. -2C_\varepsilon^{-1} B_\varepsilon^{-1} C_\varepsilon x_\varepsilon r_\varepsilon^T \left(C_\varepsilon^{-1} D_\varepsilon\right)^T \right) y,
\end{aligned}$$

so $\|M_{\phi'}^T\|_2^2 = \|M_\varepsilon\|_2$ with

$$M_\varepsilon = \gamma_\varepsilon C_\varepsilon^{-1} D_\varepsilon \left(C_\varepsilon^{-1} D_\varepsilon\right)^T + \|r_\varepsilon\|_2^2 C_\varepsilon^{-1} B_\varepsilon^{-1} \left(C_\varepsilon^{-1} B_\varepsilon^{-1}\right)^T - 2C_\varepsilon^{-1} B_\varepsilon^{-1} C_\varepsilon x_\varepsilon r_\varepsilon^T \left(C_\varepsilon^{-1} D_\varepsilon\right)^T. \tag{21}$$

Replacing D_ε by $B_\varepsilon^{-1}(A_\varepsilon^T + 2\frac{C_\varepsilon x_\varepsilon r_\varepsilon^T}{\gamma_\varepsilon})$, using $A_\varepsilon^T r_\varepsilon (C_\varepsilon x_\varepsilon)^T = -\bar{\lambda}_{n+1} C_\varepsilon x_\varepsilon (C_\varepsilon x_\varepsilon)^T$ and $\|r_\varepsilon\|_2^2 = \bar{\lambda}_{n+1}\gamma_\varepsilon$, Equation (21) simplifies to

$$M_\varepsilon = \gamma_\varepsilon C_\varepsilon^{-1} B_\varepsilon^{-1} \left(A_\varepsilon^T A_\varepsilon + \bar{\lambda}_{n+1} \left(I - 2\frac{C_\varepsilon x_\varepsilon (C_\varepsilon x_\varepsilon)^T}{\gamma_\varepsilon} \right) \right) B_\varepsilon^{-1} C_\varepsilon^{-1}.$$

Combining Equation (21) with $\varepsilon \to 0$, we have

$$
\begin{aligned}
M &= \gamma B^{-1}A^TAB^{-1} + \|r\|_2^2B^{-2} + 2\frac{\gamma}{\bar{\gamma}}B^{-1}A^Trx^TCB^{-1} \\
&\quad + 2B^{-1}\left(\frac{\gamma}{\bar{\gamma}}Cxr^TA - Cxr^TA\right)B^{-1} + 4B^{-1}\left(\frac{\gamma}{\bar{\gamma}^2}Cxr^Trx^TC - \frac{1}{\bar{\gamma}}Cxr^Trx^TC\right)B^{-1} \\
&= \gamma B^{-1}A^TAB^{-1} + \|r\|_2^2B^{-2} + 2\frac{\gamma}{\bar{\gamma}}(I - B^{-1}A^TA)xx^TCB^{-1} \\
&\quad + 2B^{-1}\left(\frac{\gamma}{\bar{\gamma}}Cxx^T(I - B^{-1}A^TA)^T - Cxx^T(I - B^{-1}A^TA)^T\right) \\
&\quad + 4\|r\|_2^2B^{-1}\left(\frac{\gamma}{\bar{\gamma}^2}Cxx^TC - \frac{1}{\bar{\gamma}}Cxx^TC\right)B^{-1} \\
&= \gamma B^{-1}A^TAB^{-1} + \|r\|_2^2B^{-2} + 2\frac{\gamma}{\bar{\gamma}}(I - B^{-1}A^TA)xx^TCB^{-1} \\
&\quad - 2\tilde{\sigma}^2B^{-1}\left(2\frac{\gamma}{\bar{\gamma}}Cxx^TC - Cxx^TC\right)B^{-1} + 4\tilde{\sigma}^2\bar{\gamma}B^{-1}\left(\frac{\gamma}{\bar{\gamma}^2}Cxx^TC - \frac{1}{\bar{\gamma}}Cxx^TC\right)B^{-1} \\
&= \gamma B^{-1}A^TAB^{-1} + \|r\|_2^2B^{-2} - 2\tilde{\sigma}^2B^{-1}Cxx^TCB^{-1} \\
&= \gamma B^{-1}\left(A^TA + \tilde{\sigma}^2\bar{\gamma}\left(I - 2\frac{Cxx^TC}{\bar{\gamma}}\right)\right)B^{-1},
\end{aligned}
$$

where we use the following results: $B^{-1}A^Tr = (I - B^{-1}A^TA)x, I - B^{-1}A^TA = -\tilde{\sigma}^2B^{-1}C, \|r\|_2^2 = \tilde{\sigma}^2\bar{\gamma}, \bar{\gamma} = 1 + \|Cx\|_2^2$, and $\gamma = 1 + \|x\|_2^2$; then, the results happen. □

3.2 | Mixed and componentwise condition numbers

When the data are badly scaled and sparse, normwise condition numbers allow large relative perturbations on small entries and may give overestimated bounds. Instead of measuring perturbations by norms, a componentwise condition number is more suitable because it measures perturbation errors for each component of the input data. Therefore, the mixed, componentwise condition numbers for the MTLS problem are worth studying. The following theorem presents the mixed and componentwise condition numbers in combination with the author's assertion in the work of Zheng et al.[16]

Theorem 3. *Let $H(A, b)$ be defined as in Lemma 1 and assume that genericity assumption (3) holds. Then, the mixed and componentwise condition number of x of the MTLS solution is expressed by*

$$\kappa^{\text{mix}}(x_{\text{MTLS}}, A, b) = \frac{\| |H(A, b)|\text{vec}([|A|, |b|])\|_\infty}{\|x\|_\infty}, \tag{22}$$

and

$$\kappa^{\text{com}}(x_{\text{MTLS}}, A, b) = \left\| \frac{|H(A, b)|\text{vec}([|A|, |b|])}{x} \right\|_\infty. \tag{23}$$

Proof. In the work of Zheng et al.,[16] Remark 4.2 shows us that the upper bounds of the mixed and componentwise condition numbers for the TLS problem given by Zhou et al.[17] and Li et al.[18] are actual condition numbers. Xie et al.[19] indicates that the condition numbers derived, respectively, in the works of Zhou et al.,[17] Li et al.,[18] and Baboulin et al.[20] are mathematically equivalent. With the same way, we know that formulae (22) and (23) are just the mixed and componentwise condition numbers for the MTLS problem, respectively. As for how to derive $H(A, b)$, see Lemma 1. □

Comment 1. We know that if $n_1 = 0$, the MTLS problem will reduce to an TLS problem, whereas if $n_2 = 0$, it will become an LS problem, which means that the TLS problem and the LS problem are two special cases of the MTLS problem (1). Therefore, it is easy to know that the normwise, mixed, and componentwise condition numbers of the TLS problem and the LS problem are unified in the ones of the MTLS problem by the expressions M and $H(A, b)$; see the details in other works.[17–22]

Remark 1. Although the expressions of the condition numbers presented are explicit, they involve the solution and their computation is intensive when the problem size is large. Thus, practical algorithms for approximating the condition numbers are worth studying. We propose statistical algorithms by taking advantage of the superiority of the small-sample statistical condition estimation (SCE) techniques; see the details in other works.[19,23–25]

4 | PERTURBATION ANALYSIS OF THE MTLS SOLUTION

Perturbation analysis is an important research area in numerical analysis. Given a problem, the condition number measures the worst-case sensitivity of its solution to small perturbations in the input data. Using it with backward error estimate, we can derive an approximate upper bound for the forward error, that is, the difference between a perturbed solution and the exact solution. In this section, we first consider the first-order perturbation bound of the MTLS solution based on the normwise condition number. For $\frac{\|\Delta x\|_2}{\|x\|_2}$, the upper bound is expressed by

$$\frac{\|\Delta x\|_2}{\|x\|_2} \leq \|M\|_2^{\frac{1}{2}} \frac{\|[A,b]\|_F}{\|x\|_2} \frac{\|[\Delta A, \Delta b]\|_F}{\|[A,b]\|_F} = \kappa^{\mathrm{rel}}(x_{\mathrm{MTLS}}, A, b) \frac{\|[\Delta A, \Delta b]\|_F}{\|[A,b]\|_F} \equiv B_{\mathrm{BY}}, \tag{24}$$

where M is the $n \times n$ matrix $M = \gamma B^{-1}\left(A^T A + \tilde{\sigma}^2 \bar{\gamma}\left(I - 2\frac{Cxx^T C}{\bar{\gamma}}\right)\right) B^{-1}$.

In addition, we find that computing the matrix cross product $A^T A$ for the normwise condition number is a source of rounding errors and is potentially numerically unstable. In order to overcome these difficulties, we present a perturbation bound for computing more effectively without using the condition number. Before deriving the explicit expression, we give a useful expansion of the smallest singular value of the perturbed matrix in terms of the smallest singular value of the original matrix.

Lemma 2 (See the work of Xie et al.[19]).
Let $\sigma_{\min}$ be the smallest nonzero and simple singular value of a matrix A with $u_{\min}$ and $v_{\min}$ being its corresponding left and right singular vectors, respectively. If ΔA is sufficiently small, then the smallest nonzero singular value $\tilde{\sigma}_{\min}$ of the perturbed matrix $\tilde{A} = A + \Delta A$ is simple and

$$\tilde{\sigma}_{\min} = \sigma_{\min} + u_{\min}^T \Delta A v_{\min} + \mathcal{O}\left(\|\Delta A\|_F^2\right). \tag{25}$$

Then, the following lemma is easy to get.

Lemma 3. *Consider the WTLS problem (5) and assume that condition (3) and assumption (6) hold. If $[A_\varepsilon, b]$ is perturbed to $[A_\varepsilon + \Delta A_\varepsilon, b + \Delta b]$, then we have*

$$\bar{\sigma}_{n+1} \bar{u}_{n+1}^T [\Delta A_\varepsilon, \Delta b] \bar{v}_{n+1} = \frac{r_\varepsilon^T (\Delta b - \Delta A_\varepsilon C_\varepsilon x_\varepsilon)}{1 + \|C_\varepsilon x_\varepsilon\|_2^2},$$

where $r_\varepsilon = b - A_\varepsilon C_\varepsilon x_\varepsilon$, $(\bar{\sigma}_{n+1}, \bar{u}_{n+1}, \bar{v}_{n+1})$ is the smallest singular triplet of the matrix (A_ε, b).

The perturbation bound for the WTLS problem is presented as follows, whose derivation is the same as the result (3.8) in the work of Xie et al.[19]

Theorem 4. *Consider the WTLS problem (5) and assume that condition (3) and assumption (6) hold. If $\|[\Delta A_\varepsilon, \Delta b]\|_F$ is sufficiently small, then we have*

$$\frac{\|\Delta x_\varepsilon\|_2}{\|x_\varepsilon\|_2} \lesssim \left(\left\|C_\varepsilon^{-1} B_\varepsilon^{-1}\right\|_2 \frac{\|r_\varepsilon\|_2 \|\Delta A_\varepsilon\|_2}{\|x_\varepsilon\|_2} + \left\|C_\varepsilon^{-1} B_\varepsilon^{-1} A_\varepsilon^T\right\|_2 \|\Delta A_\varepsilon C_\varepsilon\|_2 + \left\|C_\varepsilon^{-1} B_\varepsilon^{-1} A_\varepsilon^T\right\|_2 \frac{\|\Delta b\|_2}{\|x_\varepsilon\|_2} \right).$$

Now, we can get the upper bound for $\frac{\|\Delta x\|_2}{\|x\|_2}$ of the MTLS problem (1) by the relationship between x and x_ε, as shown in (8).

Theorem 5. *Consider the MTLS problem (1) and assume that genericity condition (3) holds. If $\|[\Delta A, \Delta b]\|_F$ is sufficiently small, then we have*

$$\frac{\|\Delta x\|_2}{\|x\|_2} \lesssim \|B^{-1}\|_2 \frac{\|r\|_2 \|\Delta A\|_2}{\|x\|_2} + \|B^{-1} A^T\|_2 \|\Delta A\|_2 + \|B^{-1} A^T\|_2 \frac{\|\Delta b\|_2}{\|x\|_2}. \tag{26}$$

Proof. By (8), we know $\lim_{\varepsilon \to 0^+} x_\varepsilon = x$, then $\lim_{\varepsilon \to 0^+} \Delta x_\varepsilon = \Delta x$,

$$\begin{aligned} \frac{\|\Delta x\|_2}{\|x\|_2} &= \lim_{\varepsilon \to 0^+} \frac{\|\Delta x_\varepsilon\|_2}{\|x_\varepsilon\|_2} \\ &\lesssim \lim_{\varepsilon \to 0^+} \left(\left\|C_\varepsilon^{-1} B_\varepsilon^{-1} C_\varepsilon^{-1}\right\|_2 \frac{\|\Delta A\|_2 \|r_\varepsilon\|_2}{\|x_\varepsilon\|_2} + \left\|C_\varepsilon^{-1} B_\varepsilon^{-1} A_\varepsilon^T\right\|_2 \|\Delta A_\varepsilon C_\varepsilon\|_2 + \left\|C_\varepsilon^{-1} B_\varepsilon^{-1} A_\varepsilon^T\right\|_2 \frac{\|\Delta b\|_2}{\|x_\varepsilon\|_2} \right) \\ &= \left(\|B^{-1}\|_2 \frac{\|r\|_2 \|\Delta A\|_2}{\|x\|_2} + \|B^{-1} A^T\|_2 \|\Delta A\|_2 + \|B^{-1} A^T\|_2 \frac{\|\Delta b\|_2}{\|x\|_2} \right). \end{aligned}$$

□

As for the two terms $\|B^{-1}A^T\|_2$ and $\|B^{-1}\|_2$ involved in (26), one can adopt the power method or the SCE to estimate them; see the work of Xie et al.[19] for details. From Proposition 3.2 in the work of Xie et al.,[19] we have that the bound obtained in (26) is sharper than the upper bounds in (24) if $\Delta A = 0 \in \mathbb{R}^{m\times n}$.

Wei et al.[12] gives an upper bound of the solution for the MTLS problem under the assumption that the perturbation of A_1 is much smaller than that of A_2 and that the perturbation of $[A, b]$ is small enough. We find that the quality of the bounds he gives depends on the value of $\tilde{\sigma}$, whereas our results depend on the size of the perturbation to the data largely. We compare our results with Wei's by giving examples.

5 | CONNECTIONS BETWEEN THE MTLS AND LS SOLUTIONS

Comparing MTLS solution (4) with the LS solution shows that σ, $\tilde{\sigma}$, and C determine the differences between both solutions, in a sense, that we could say that σ, $\tilde{\sigma}$, and C measure the difference between both solutions, as well as the degree of incompatibility of the set $Ax \approx b$, which is exactly expressed below.

Theorem 6. *Let x_{MTLS} be the solution of the MTLS problem (1), and let x_{LS} be the solution of the LS problem $Ax \approx b$. Then, under condition (3), we have the following estimates:*

$$\begin{aligned} x_{\mathrm{MTLS}} - x_{\mathrm{LS}} &= \tilde{\sigma}^2 \begin{pmatrix} 0 & -R_{11}^{-1}R_{12} \\ 0 & I \end{pmatrix} \begin{pmatrix} I & 0 \\ 0 & \left(R_{22}^T R_{22} - \tilde{\sigma}^2 I\right)^{-1} R_{22}^{\dagger} \end{pmatrix} Q^T b, \\ \frac{\tilde{\sigma}^2}{\sigma(\sigma^2 - \tilde{\sigma}^2)}\|b\|_2 \le \|x_{\mathrm{MTLS}} &- x_{\mathrm{LS}}\|_2 \le \frac{\tilde{\sigma}^2}{\sigma(\sigma^2 - \tilde{\sigma}^2)}\sqrt{1+\acute{\sigma}^2}\|b\|_2, \\ \|x_{\mathrm{MTLS}}\|_2 &\ge \|x_{\mathrm{LS}}\|_2, \end{aligned} \tag{27}$$

where σ, $\tilde{\sigma}$ are defined in Equation (3) and $\acute{\sigma}$ is the maximum singular value of the matrix $R_{11}^{-1}R_{12}$.

Proof. From (8), we know

$$\begin{aligned} x_{\mathrm{WTLS}} &= C_\varepsilon^{-1}\left(A_\varepsilon^T A_\varepsilon - \bar{\sigma}_{n+1}^2 I\right)^{-1} A_\varepsilon^T b \\ &= C_\varepsilon^{-1}\left(A_\varepsilon^T A_\varepsilon - \bar{\sigma}_{n+1}^2 I\right)^{-1} A_\varepsilon^T A_\varepsilon C_\varepsilon x_{\mathrm{WLS}} \\ &= C_\varepsilon^{-1}\left(I - \bar{\sigma}_{n+1}^2\left(A_\varepsilon^T A_\varepsilon\right)^{-1}\right)^{-1} C_\varepsilon x_{\mathrm{WLS}} \\ &= C_\varepsilon^{-1}\left(I + \bar{\sigma}_{n+1}^2\left(A_\varepsilon^T A_\varepsilon - \bar{\sigma}_{n+1}^2 I\right)^{-1}\right) C_\varepsilon x_{\mathrm{WLS}}. \end{aligned}$$

Then, we have

$$\begin{aligned} x_{\mathrm{MTLS}} - x_{\mathrm{LS}} &= \lim_{\varepsilon\to 0^+}(x_{\mathrm{WTLS}} - x_{\mathrm{WLS}}) \\ &= \lim_{\varepsilon\to 0^+} C_\varepsilon^{-1}\bar{\sigma}_{n+1}^2\left(A_\varepsilon^T A_\varepsilon - \bar{\sigma}_{n+1}^2 I\right)^{-1} C_\varepsilon x_{\mathrm{WLS}} \\ &= \lim_{\varepsilon\to 0^+} C_\varepsilon^{-1}\bar{\sigma}_{n+1}^2\left(A_\varepsilon^T A_\varepsilon - \bar{\sigma}_{n+1}^2 I\right)^{-1} C_\varepsilon^{-1} C_\varepsilon^2 x_{\mathrm{WLS}} \\ &= \tilde{\sigma}^2 (A^T A - \tilde{\sigma}^2 C)^{-1} C x_{\mathrm{LS}} \\ &= \tilde{\sigma}^2 \begin{pmatrix} 0 & -R_{11}^{-1}R_{12}\left(R_{22}^T R_{22} - \tilde{\sigma}^2 I\right)^{-1} \\ 0 & \left(R_{22}^T R_{22} - \tilde{\sigma}^2 I\right)^{-1} \end{pmatrix} C (A^T A)^{-1} A^T b \\ &= \tilde{\sigma}^2 \begin{pmatrix} 0 & -R_{11}^{-1}R_{12}\left(R_{22}^T R_{22} - \tilde{\sigma}^2 I\right)^{-1} \\ 0 & \left(R_{22}^T R_{22} - \tilde{\sigma}^2 I\right)^{-1} \end{pmatrix} C \begin{pmatrix} R_{11}^T R_{11} & R_{11}^T R_{12} \\ R_{12}^T R_{11} & R_{12}^T R_{12} + R_{22}^T R_{22} \end{pmatrix}^{-1} \\ &\quad \cdot \begin{pmatrix} R_{11}^T & 0 \\ R_{12}^T & R_{22}^T \end{pmatrix} Q^T b \\ &= \tilde{\sigma}^2 \begin{pmatrix} 0 & -R_{11}^{-1}R_{12}\left(R_{22}^T R_{22} - \tilde{\sigma}^2 I\right)^{-1} \\ 0 & \left(R_{22}^T R_{22} - \tilde{\sigma}^2 I\right)^{-1} \end{pmatrix} C \begin{pmatrix} R_{11}^{-1} & -R_{11}^{-1}R_{12}R_{22}^{\dagger} \\ 0 & R_{22}^{\dagger} \end{pmatrix} Q^T b \\ &= \tilde{\sigma}^2 \begin{pmatrix} 0 & -R_{11}^{-1}R_{12}\left(R_{22}^T R_{22} - \tilde{\sigma}^2 I\right)^{-1} R_{22}^{\dagger} \\ 0 & \left(R_{22}^T R_{22} - \tilde{\sigma}^2 I\right)^{-1} R_{22}^{\dagger} \end{pmatrix} Q^T b \\ &= \tilde{\sigma}^2 \begin{pmatrix} 0 & -R_{11}^{-1}R_{12} \\ 0 & I \end{pmatrix} \begin{pmatrix} I & 0 \\ 0 & \left(R_{22}^T R_{22} - \tilde{\sigma}^2 I\right)^{-1} R_{22}^{\dagger} \end{pmatrix} Q^T b, \end{aligned}$$

and consequently,

$$\begin{aligned}\|x_{\mathrm{MTLS}}-x_{\mathrm{LS}}\|_2 &= \left\| \tilde{\sigma}^2 \begin{pmatrix} 0 & -R_{11}^{-1}R_{12} \\ 0 & I \end{pmatrix} \begin{pmatrix} I & 0 \\ 0 & \left(R_{22}^T R_{22}-\tilde{\sigma}^2 I\right)^{-1} R_{22}^{\dagger} \end{pmatrix} Q^T b \right\|_2 \\ &\le \tilde{\sigma}^2 \left\| \begin{pmatrix} 0 & -R_{11}^{-1}R_{12} \\ 0 & I \end{pmatrix} \begin{pmatrix} I & 0 \\ 0 & \left(R_{22}^T R_{22}-\tilde{\sigma}^2 I\right)^{-1} R_{22}^{\dagger} \end{pmatrix} \right\|_2 \|Q^T b\|_2 \\ &\le \frac{\tilde{\sigma}^2}{\sigma(\sigma^2-\tilde{\sigma}^2)} \left\| \begin{pmatrix} -R_{11}^{-1}R_{12} \\ I \end{pmatrix} \right\|_2 \|b\|_2 \\ &= \frac{\tilde{\sigma}^2}{\sigma(\sigma^2-\tilde{\sigma}^2)} \sqrt{1+\acute{\sigma}^2}\, \|b\|_2.\end{aligned}$$

It is easy to know that

$$\frac{\tilde{\sigma}^2}{\sigma(\sigma^2-\tilde{\sigma}^2)}\|b\|_2 \le \|x_{\mathrm{MTLS}}-x_{\mathrm{LS}}\|_2,$$

where $\acute{\sigma}$ is the maximum singular value of $R_{11}^{-1}R_{12}$. We know, from the work of Van Huffel et al.,[26] that $\|x_{\mathrm{WTLS}}\|_2 \ge \|x_{\mathrm{WLS}}\|_2$. On the other hand, because $\lim_{\epsilon\to 0^+} x_{\mathrm{WTLS}} = x_{\mathrm{MTLS}}$, $\lim_{\epsilon\to 0^+} x_{\mathrm{WLS}} = x_{\mathrm{LS}}$, there comes $\|x_{\mathrm{MTLS}}\|_2 \ge \|x_{\mathrm{LS}}\|_2$. □

The upper bound is met whenever $\hat{U}(Q^T b)_2 // \acute{u}_{n_2}$, where $\acute{u}_{n_2}$ means the left singular vector of the minimal singular value σ of R_{22}, $\hat{U}$ consists of the left singular vector of A, and $a = (a_1{}^T, a_2{}^T)^T$ with $a_2 \in R^{n_2}$.

The main contribution of Theorem 6 lies in the fact that it points out the parameters σ, $\tilde{\sigma}$, C and the orientation of A, b with respect to $\acute{u}_{n_2}$, which mainly influence the expected differences in accuracy between the MTLS and the LS solutions of the set $Ax \approx b$ in the presence of perturbations in the measurements A and b. As $\tilde{\sigma}$ deviates from zero, the set $Ax \approx b$ becomes more and more incompatible and the differences between the LS and the MTLS solutions are more and more pronounced. In a sense, we could say that σ, $\tilde{\sigma}$, and C measure the difference between both solutions. In addition, the result of Theorem 6 extends and simplifies Liu's results[10] about distance between the MTLS and the LS solutions.

These parameters also describe the connections between the MTLS residual r_{MTLS} and the LS residual r_{LS} in the following.

Theorem 7. *Let r_{MTLS} be the MTLS residual (1), and let r_{LS} be the LS residual of the LS problem $Ax \approx b$. Then, under condition (3), we have the following estimates:*

$$\begin{aligned}\|r_{\mathrm{MTLS}}-r_{\mathrm{LS}}\|_2 &\le \frac{\tilde{\sigma}^2}{\sigma(\sigma^2-\tilde{\sigma}^2)}\grave{\sigma}\|b\|_2, \\ \|r_{\mathrm{MTLS}}\|_2 &\ge \|r_{\mathrm{LS}}\|_2,\end{aligned} \tag{28}$$

where σ, $\tilde{\sigma}$ are defined in Equation (3) and $\grave{\sigma}$ is the maximum singular value of the matrix R_{22}.

Proof. Because $r_{\mathrm{MTLS}} - r_{\mathrm{LS}} = A(x_{\mathrm{MTLS}} - x_{\mathrm{LS}})$, we obtain

$$\begin{aligned}r_{\mathrm{MTLS}}-r_{\mathrm{LS}} &= \tilde{\sigma}^2 A(A^TA-\tilde{\sigma}^2 C)^{-1} C x_{\mathrm{LS}} \\ &= \tilde{\sigma}^2 (A_1, A_2) \begin{pmatrix} 0 & -R_{11}^{-1}R_{12} \\ 0 & I \end{pmatrix} \begin{pmatrix} I & 0 \\ 0 & \left(R_{22}^T R_{22}-\tilde{\sigma}^2 I\right)^{-1} \end{pmatrix} C x_{\mathrm{LS}} \\ &= \tilde{\sigma}^2 (A_1, A_2) \begin{pmatrix} 0 & -A_1^{\dagger}A_2 \\ 0 & I \end{pmatrix} \begin{pmatrix} I & 0 \\ 0 & \left(R_{22}^T R_{22}-\tilde{\sigma}^2 I\right)^{-1} \end{pmatrix} C x_{\mathrm{LS}} \\ &= \tilde{\sigma}^2 \begin{pmatrix} 0 & \left(-A_1A_1^{\dagger}A_2 + A_2\right)\left(R_{22}^T R_{22}-\tilde{\sigma}^2 I\right)^{-1} \end{pmatrix} \begin{pmatrix} 0 & 0 \\ 0 & R_{22}^{\dagger} \end{pmatrix} Q^T b, \\ &= \tilde{\sigma}^2 \begin{pmatrix} 0 & \left(-A_1A_1^{\dagger}A_2 + A_2\right)\left(R_{22}^T R_{22}-\tilde{\sigma}^2 I\right)^{-1} R_{22}^{\dagger} \end{pmatrix} Q^T b,\end{aligned}$$

taking norms

$$
\begin{aligned}
\|r_{\mathrm{MTLS}} - r_{\mathrm{LS}}\|_2 &= \left\| \tilde{\sigma}^2 \begin{pmatrix} 0 & \left(-A_1A_1^{\dagger}A_2 + A_2\right)\left(R_{22}^T R_{22} - \tilde{\sigma}^2 I\right)^{-1} R_{22}^{\dagger} \end{pmatrix} Q^T b \right\|_2 \\
&\leq \tilde{\sigma}^2 \left\| \begin{pmatrix} 0 & \left(-A_1A_1^{\dagger}A_2 + A_2\right)\left(R_{22}^T R_{22} - \tilde{\sigma}^2 I\right)^{-1} R_{22}^{\dagger} \end{pmatrix} \right\|_2 \|b\|_2 \\
&= \tilde{\sigma}^2 \left\| \begin{pmatrix} 0 & Q \begin{pmatrix} 0 \\ R_{22} \end{pmatrix} \left(R_{22}^T R_{22} - \tilde{\sigma}^2 I\right)^{-1} R_{22}^{\dagger} \end{pmatrix} \right\|_2 \|b\|_2 \\
&\leq \frac{\tilde{\sigma}^2}{\sigma(\sigma^2 - \tilde{\sigma}^2)} \grave{\sigma} \|b\|_2,
\end{aligned}
$$

where $\grave{\sigma}$ is the maximum singular value of the matrix R_{22}. Finally, because the LS always minimizes any orthogonally invariant norm of its residual, (28) follows immediately. □

Remark 2. In this section, the MTLS technique is compared analytically with the classical LS method. With algebraic connections between their solutions, their residuals applied to the fitting of the data are proved. They all reveal that the same parameters (σ, $\tilde{\sigma}$, and C) mainly determine the correspondences and differences between both techniques. These parameters are, moreover, useful tools for getting more insight into the sensitivity of both techniques with respect to perturbations.

6 | NUMERICAL EXAMPLES

In this section, we give numerical examples to check our results. The following numerical tests are performed via MATLAB R2015a with machine precision $\mu = 2.22\mathrm{e}-16$ in a laptop with Intel Core (TM)2 Duo CPU by using double precision.

Example 1. Take m = 100, n = 60, $n_1 = 30$, $n_2 = 30$. Choose 0 as the rand seed and use command rand in MATLAB to generate a random $m \times n$ matrix A with a uniform distribution on the interval (0,1).

(1) Choose 1 as the rand seed and generate a random vector b in MATLAB. Then, $\sigma^2 = 9.88\mathrm{e}-1$, $\tilde{\sigma}^2 = 8.38e-1$, $\tilde{\sigma}^2/\tilde{\sigma}_-^2 = 0.85$, where $\tilde{\sigma}_-^2$ is the second smallest singular value of (R_{22}, R_{2b}). The MTLS problem is well conditioned.
(2) Let $b = 1_m$ be an all-1 vector. Then, $\sigma^2 = 9.88\mathrm{e}-1$, $\tilde{\sigma}^2 = 1.89e-1$, $\tilde{\sigma}^2/\tilde{\sigma}_-^2 = 0.19$. Therefore, the MTLS problem is well conditioned.

This example illustrates how the ratio $\tilde{\sigma}/\tilde{\sigma}_-$ affects the forward error and the perturbation bounds. In Table 1, we compare the exact relative error about the MTLS solution with the upper bounds (26) and the above bounds B_{BY} derived from (24). We find that when the ratio $\tilde{\sigma}/\tilde{\sigma}_-$ is larger, the perturbation bounds estimate the relative error better. Compared with the upper bound of the relative error, which we name B_{Wei} here, given in Theorem 4.2 of the work of Wei et al.,[12] our results are obviously better. In addition, we give the exact relative error about the smallest singular value of $[A_\varepsilon, b]$.

Example 2. In order to test the effect of the MTLS algorithm and its related results further, the experimental data in the work of Siping et al.[27] are cited, and the coordinate observations are listed in Table 2.

Coordinate transformation is the process of transforming spatial data from one coordinate system to another. In essence, it is the process of solving coordinate transformation parameters according to common known points in two coordinate systems. The transformation parameters of the two coordinate systems include three translation parameters, one scale parameters, and three rotation parameters. When the rotation angle is small or the initial value is known, the rotation

TABLE 1 Comparisons of forward error and upper bounds for a perturbed mixed least squares–total least squares (MTLS) problem and the relative condition number of the MTLS problem

b	$\frac{\|\tilde{x}-x\|_2}{\|x\|_2}$	(26)	B_{BY}	B_{Wei}	$\frac{\|\tilde{\rho}-\rho\|_2}{\|\rho\|_2}$
rand(m,1)	2.609047e−09	9.726393e−8	7.412667e−7	5.043150e−04	1.0203e−09
ones(m,1)	4.1806e−11	4.34547e−9	3.05349e−8	2.26601e−05	2.3019e−11

TABLE 2 Coordinate observations of control points and their corresponding accuracy (unit: m)

	Original coordinates			Target coordinates		
	X_s	Y_s	Z_s	X_t	Y_t	Z_t
1	−2,802,191.3482	5,009,064.7657	2,772,381.1768	−2,802,088.4182	5,009,123.1569	2,772,386.5699
2	−2,810,175.6515	5,016,086.1120	2,751,955.0531	−2,810,072.7309	5,016,144.5721	2,751,960.5007
3	−2,820,567.2272	5,009,905.3444	2,752,470.3858	−2,820,464.3942	5,009,963.9917	2,752,475.9211
4	−2,817,162.6538	5,002,454.3520	2,769,299.1106	−2,817,059.8351	5,002,512.9993	2,769,304.6288
5	−2,825,775.8182	4,995,785.4955	2,772,390.1695	−2,825,673.0906	4,995,844.3013	2,772,395.7629
6	−2,821,096.7634	4,981,344.2112	2,802,869.4944	−2,820,994.0605	4,981,403.0486	2,802,875.0773
7	−2,824,710.6654	4,984,669.2846	2,793,431.9999	−2,824,607.9846	4,984,728.1458	2,793,437.5997
8	−2,827,287.5380	4,983,602.6974	2,792,671.0817	−2,827,184.8759	4,983,661.6016	2,792,676.7042
9	−2,759,256.9584	5,019,419.0725	2,796,705.2762	−2,759,153.7202	5,019,476.8036	2,796,710.3167
10	−2,800,063.3339	5,001,135.2900	2,788,830.1959	−2,799,960.4176	5,001,193.7094	2,788,835.5802
11	−2,841,162.8707	4,981,982.5041	2,781,464.4489	−2,841,060.2902	4,982,041.6183	2,781,470.1805

TABLE 3 Comparisons of forward error and upper bounds for a perturbed problem with different methods

$\lVert[\Delta A, \Delta b]\rVert_F$	Methods	$\frac{\lVert\Delta x_M\rVert_2}{\lVert x_M\rVert_2}$	Upper bounds		$\lVert[\Delta A, \Delta b]\rVert_F$	Methods	$\frac{\lVert\Delta x_M\rVert_2}{\lVert x_M\rVert_2}$	Upper bounds	
1e−9	LS	8.548845e−09	[22]:	2.764840e−07	1e−5	LS	4.536314e−05	[22]:	2.604783e−03
	MTLS	4.704303e−09	(24):	2.764841e−08		MTLS	4.528094e−05	(24):	2.704783e−03
			(26):	2.721328e−08				(26):	2.636841e−03
	TLS	2.034037e−08	[19]:	2.835150e−07		TLS	4.598858e−05	[19]:	2.773566e−03
1e−8	LS	6.995074e−08	[22]:	3.185115e−06	1e−3	LS	1.062318e−02	[22]:	3.238308e−01
	MTLS	3.543272e−08	(24):	3.285115e−07		MTLS	1.032313e−02	(24):	3.238308e−01
			(26):	3.132299e−07				(26):	3.118040e−01
	TLS	2.972459e−07	[19]:	3.266113e−06		TLS	1.068807e−02	[19]:	3.320658e−01

Note. LS = least squares; MTLS = mixed least squares–total least squares.

TABLE 4 Comparisons of forward error and upper bounds for a perturbed problem with different methods

n_1	0 (TLS)	100	250	300	400	499	500 (LS)
cond	1.006244e+00	2.684769e+02	4.968268e+08	7.263737e+05	4.018006e+04	1.006244+00	1.006761e+00
$\frac{\lVert\Delta x_M\rVert_2}{\lVert x_M\rVert_2}$	1.378771e−11	7.011533e−10	6.971499e−09	3.768612e−10	2.093946e−10	1.383191e−11	1.926994e−11
B_{BY}	6.989267e−10	1.974395e−09	2.517398e−05	3.322717e−07	5.852934-08	6.98267e−10	7.038612e−10
Upper bounds	–	5.771529e−08	9.668754e−04	9.088216e−07	8.402465e−07	5.392393e−10	–

Note. TLS = total least squares; LS = least squares.

matrix composed of three rotation angles can be simplified, and the space rectangular coordinates can be transformed into the linear Bursa model.[27] In this example, we want to check the perturbation bounds for the linear Bursa model with random perturbation $\lVert[\Delta A, \Delta b]\rVert_F$. Define $\frac{\lVert\Delta x_M\rVert_2}{\lVert x_M\rVert_2}$ as the exact relative error. Compared with the LS method and the TLS method, the MTLS method gives a smaller relative error and a better estimate of the upper bound as the data perturbation decreases. Compared with (24), the upper bound (26) is tighter when data perturbation is smaller. Thus, Table 3 tell us that the superiority of using the MTLS method to solve the problem is explained in a more profound way.

Example 3. In this example, we consider the linear problem $Ax \approx b$, where $[A, b]$ is defined by

$$[A, b] = Y \begin{pmatrix} D \\ 0 \end{pmatrix} Z^T \in \mathbb{R}^{m\times(n+1)}, \quad Y = I_m - 2yy^T, \quad Z = I_{n+1} - 2zz^T,$$

where $y \in \mathbb{R}^m$ and $z \in \mathbb{R}^{n+1}$ are random unit vectors and $D = \operatorname{diag}(n, n-1, \dots, 1, 1-\epsilon_p)$ for a given parameter $\epsilon_p = 9.99976032\text{e} - 1$. We consider a random perturbation $\lVert[\Delta A, \Delta b]\rVert_F = 10^{-10}$, and take $m = 1{,}000, n = 500$ in this example.

Define $\frac{\lVert\Delta x_M\rVert_2}{\lVert x_M\rVert_2}$ as the exact relative error, and denote B_{BY} as the relative data perturbation. In Table 4, with the different values of n_1, the condition numbers of corresponding solutions are different. When the value of n_1 is about 250, the condition number of the solution reaches its topmost levels. With the increase of the condition numbers of solutions, the relative errors of the solutions and there upper bounds are also increased. This indicates that, the larger the ill condition of the problem is, the less reliable the first-order approach is when large perturbations are considered. We also observe that our bounds are sharp when n_1 is large enough.

7 | CONCLUSIONS

In this paper, we investigated the normwise, mixed, and componentwise condition numbers of the MTLS problem by using the point of interpreting the MTLS problem as a weighted TLS problem and find that the normwise, mixed, and componentwise condition numbers of the TLS problem and the LS problem are unified in the ones of the MTLS problem. In the analysis of the first-order perturbation, we first provide an upper bound based on the normwise condition number. In order to overcome the problems encountered in calculating the normwise condition number, we give an upper bound for computing more effectively for the MTLS problem. The type of the perturbation bound can enjoy storage and computational advantages and demonstrate its superiority by the numerical example. As two estimation techniques for solving the linear parameter estimation problems, interesting connections between their solutions, their residuals for the MTLS problem, and the LS problem are compared. They all reveal that the same parameters (σ, $\tilde{\sigma}$, and C) mainly determine the correspondences and differences between both techniques.

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