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A CONTRIBUTION TO THE CONDITIONING OF THE MIXED LEAST-SQUARES SCALED TOTAL LEAST-SQUARES PROBLEM*

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Abstract. A new closed formula for first-order perturbation estimates for the solution of the mixed least-squares scaled total least-squares (MLSSTLS) problem is presented. It is mathematically equivalent to the one by [Zhang and Wang, Numer. Algorithms, 89 (2022), pp. 1223–1246]. With this formula, new closed formulas for the relative normwise, mixed, and componentwise condition numbers of the MLSSTLS problem are derived. Compact forms and upper bounds for the relative normwise condition number are also given in order to obtain economic storage and efficient computations.

Key words. mixed least-squares scaled total least-squares, condition numbers, mixed least-squares total least-squares

AMS subject classifications. 65F20, 65F35

1. Introduction. The standard approaches to solve an overdetermined linear system $Ax \approx b$ is to find minimal corrections of the matrix A and/or the vector b such that the corrected system is consistent, such as, for instance, for the least-squares (LS) method, the data least-squares (DLS) method, and the total least-squares (TLS) method. Rao [9] proposed the scaled total least-squares (STLS) method that unifies the LS, DLS, and TLS methods. For a given $A \in \mathbb{R}^{m\times n}$ $(m \geq n)$ and $b \in \mathbb{R}^m$, based on the work of Rao, Paige, and Strakoš [8], the STLS problem is formulated as follows:

$$\min_{E,f} \left\| \begin{bmatrix} E & f \end{bmatrix} \right\|_F, \qquad \text{subject to} \quad (A+E)\lambda x = \lambda b + f,$$

where λ is a real positive parameter.

However, in many linear parameter estimation problems, some entries of the data matrix A may contain no errors. For instance, in regression analysis [2], system identification [10], and signal processing [11], some signals can be observed without error, whereas the other ones are disturbed by zero-mean white noise. These cases often result from the fact that some of the columns of A are exact. Hence, to maximize the accuracy of the estimated parameters x, the case that some of the columns in the data matrix A are error-free whereas others are perturbed is naturally encountered when estimating a parameter x using the TLS approach. The TLS problem with some exact columns in the data matrix is known as the mixed least-squares total least-squares (MTLS) problem.

Let $A = \begin{bmatrix} A_1 & A_2 \end{bmatrix}$ with $A_1 \in \mathbb{R}^{m\times n_1}$, $A_2 \in \mathbb{R}^{m\times n_2}$, and $n_1 + n_2 = n$. Assume that the columns of A_1 are known exactly and A is of full column rank. If we partition the vector $x = \begin{bmatrix} x_1^T & x_2^T \end{bmatrix}^T$, with $x_1 \in \mathbb{R}^{n_1}$ and $x_2 \in \mathbb{R}^{n_2}$, then the MTLS problem is stated as

$$\min_{E_2,f} \left\| \begin{bmatrix} E_2 & f \end{bmatrix} \right\|_F, \qquad \text{subject to} \quad A_1x_1 + (A_2+E_2)x_2 = b + f. \tag{1.1}$$

Obviously, if $n_1 = 0$, then the MTLS problem becomes the TLS problem, whereas if $n_2 = 0$, then it will reduce to the LS problem. However, the MTLS problem does not involve the

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STLS problem. Based on this observation, Zhang and Wang [13] generalized the MTLS problem (1.1) as follows:

$$\min_{E_2,f} \left\| \begin{bmatrix} E_2 & f \end{bmatrix} \right\|_F, \qquad \text{subject to} \quad A_1 x_1 + (A_2 + E_2)\lambda x_2 = \lambda b + f. \tag{1.2}$$

The authors refer to (1.2) as the mixed least-squares scaled total least-squares (MLSSTLS) problem. The vector $x = x_{\text{MS}}$ satisfying (1.2) is called the MLSSTLS solution.

Condition numbers measure the worst-case sensitivity of a solution of a problem with respect to small perturbations in the input data. The condition numbers of the TLS problem, the STLS problem, and the MTLS problem have been studied widely, e.g., by Zhou et al. [16], Baboulin and Gratton [1], Li and Jia [5, 4], Zheng et al. [14], Wang et al. [12], Zheng and Yang [15]. Recently, Zhang and Wang [13] studied a closed formula for a first-order perturbation estimate of the MLSSTLS solution and gave explicit expressions for the condition numbers of the MLSSTLS problem. We notice that the closed formulas for the normwise, mixed, and componentwise condition numbers derived in [13] are based on the evaluation of the norm of a matrix expressed as a Kronecker product, resulting in large matrices, which may be, as pointed out by the authors, impractical to compute, especially for large-scale problems. In this paper, we revisit the condition numbers for the MLSSTLS problem. We derive another different closed formula for the first-order perturbation estimate of the MLSSTLS solution and show that the formula is equivalent to that in [13]. We also present a compact form for the condition numbers which allows for a more efficient computation using less storage.

Throughout this paper, we denote by $\mathbb{R}^{m\times n}$ the space of all $m \times n$ real matrices and by $\|\cdot\|_2$, $\|\cdot\|_\infty$, and $\|\cdot\|_F$ the 2-norm, the ∞-norm, and the Frobenius norm, 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 $0_{m,n}$ is the $m \times n$ matrix with all zero entries (if no confusion occurs, we drop the subscript). For any matrix $A = \begin{bmatrix} a_1 & a_2 & \cdots & a_n \end{bmatrix} = [a_{ij}] \in \mathbb{R}^{m\times n}$ and $C \in \mathbb{R}^{p\times q}$, A^T denotes the transpose of A, and the Kronecker product $A \otimes C$ is defined as $A \otimes C = [a_{ij}C] \in \mathbb{R}^{mp\times nq}$. We define $\operatorname{vec}(A) \in \mathbb{R}^{mn}$ by $\operatorname{vec}(A) = \begin{bmatrix} a_1^T & a_2^T & \cdots & a_n^T \end{bmatrix}^T$, i.e., by stacking the columns of A.

2. Algebraic properties of the MLSSTLS problem. Let the QR decomposition of $\begin{bmatrix} A & b \end{bmatrix}$ in (1.1) be

$$Q^T \begin{bmatrix} A & b \end{bmatrix} = \begin{bmatrix} Q_1 & Q_2 \end{bmatrix}^T \begin{bmatrix} A_1 & A_2 & b \end{bmatrix} = \begin{array}{c} \\ n_1 \\ m-n_1 \end{array} \begin{array}{c} \begin{array}{ccc} n_1 & n_2 & 1 \end{array} \\ \begin{bmatrix} R_{11} & R_{12} & R_{1b} \\ 0 & R_{22} & R_{2b} \end{bmatrix} \end{array},$$

and

$$Q^T E_2 = \begin{array}{c} n_1 \\ m-n_1 \end{array} \begin{bmatrix} \bar{E}_{21} \\ \bar{E}_{22} \end{bmatrix}, \qquad Q^T f = \begin{array}{c} n_1 \\ m-n_1 \end{array} \begin{bmatrix} \bar{f}_1 \\ \bar{f}_2 \end{bmatrix},$$

where $Q_1 \in \mathbb{R}^{m\times n_1}$ and $Q_2 \in \mathbb{R}^{m\times(m-n_1)}$. Let $\sigma_k(A)$ denote the kth largest singular value of A. If

$$\hat{\sigma} := \sigma_{n_2}(R_{22}) > \sigma := \sigma_{n_2+1}\left(\begin{bmatrix} R_{22} & \lambda R_{2b} \end{bmatrix}\right) > 0, \tag{2.1}$$

then the MLSSTLS problem (1.2) has a unique solution, and it is equivalent to [13]

$$\min_{\bar{E}_{22},\bar{f}_2} \left\| \begin{bmatrix} \bar{E}_{22} & \bar{f}_2 \end{bmatrix} \right\|_F, \qquad \text{subject to} \quad (R_{22} + \bar{E}_{22})\lambda x_2 = \lambda R_{2b} + \bar{f}_2 \tag{2.2}$$

and

$$R_{11}x_1 = \lambda R_{1b} - \lambda R_{12}x_2. \tag{2.3}$$

Throughout this paper, we assume that the condition in (2.1) holds.

THEOREM 2.1. *Let* $C = \operatorname{diag}(0_{n_1}, I_{n_2})$ *and* $D = \operatorname{diag}(\lambda I_{n_1}, I_{n_2})$*, where* 0_{n_1} *is the* $n_1 \times n_1$ *zero matrix. Then the MLSSTLS solution* x_{MS} *solves the system*

$$\begin{bmatrix} A^TA & A^Tb \\ b^TA & b^Tb \end{bmatrix} \begin{bmatrix} D^{-1}x \\ -1 \end{bmatrix} = \sigma^2 \begin{bmatrix} C & 0 \\ 0 & \frac{1}{\lambda^2} \end{bmatrix} \begin{bmatrix} D^{-1}x \\ -1 \end{bmatrix}, \tag{2.4}$$

where σ *is defined in* (2.1).

Proof. The solution x_2 of (2.2) satisfies the augmented system

$$\begin{bmatrix} R_{22}^TR_{22} & \lambda R_{22}^TR_{2b} \\ \lambda R_{2b}^TR_{22} & \lambda^2 R_{2b}^TR_{2b} \end{bmatrix} \begin{bmatrix} \lambda x_2 \\ -1 \end{bmatrix} = \sigma^2 \begin{bmatrix} \lambda x_2 \\ -1 \end{bmatrix}.$$

Combining this with equality (2.3), we have

$$\begin{bmatrix} R_{11}^TR_{11} & R_{11}^TR_{12} & \lambda R_{11}^TR_{1b} \\ 0 & R_{22}^TR_{22} & \lambda R_{22}^TR_{2b} \\ 0 & \lambda R_{2b}^TR_{22} & \lambda^2 R_{2b}^TR_{2b} \end{bmatrix} \begin{bmatrix} x_1 \\ \lambda x_2 \\ -1 \end{bmatrix} = \sigma^2 \begin{bmatrix} 0 \\ \lambda x_2 \\ -1 \end{bmatrix}.$$

According to the QR decomposition of $\begin{bmatrix} A & b \end{bmatrix}$ and (2.3), the above equality can be rewritten as

$$\begin{bmatrix} A_1^TA_1 & A_1^TA_2 & \lambda A_1^Tb \\ A_2^TA_1 & A_2^TA_2 & \lambda A_2^Tb \\ \lambda b^TA_1 & \lambda b^TA_2 & \lambda^2 b^Tb \end{bmatrix} \begin{bmatrix} x_1 \\ \lambda x_2 \\ -1 \end{bmatrix} = \sigma^2 \begin{bmatrix} C & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 0 \\ \lambda x_2 \\ -1 \end{bmatrix},$$

which is equivalent to

$$\operatorname{diag}(\lambda I_n, \lambda^2) \begin{bmatrix} A_1^TA_1 & A_1^TA_2 & A_1^Tb \\ A_2^TA_1 & A_2^TA_2 & A_2^Tb \\ b^TA_1 & b^TA_2 & b^Tb \end{bmatrix} \begin{bmatrix} D^{-1}x \\ -1 \end{bmatrix} = \sigma^2 \begin{bmatrix} C & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 0 \\ \lambda x_2 \\ -1 \end{bmatrix}.$$

By premultiplying the above equality by the inverse matrix of $\operatorname{diag}(\frac{1}{\lambda}I_n, \frac{1}{\lambda^2})$ from the left, we obtain (2.4). ∎

REMARK 2.2. According to Theorem 2.1, the unique MLSSTLS solution x_{MS} can be expressed as

$$x_{\text{MS}} = D(A^TA - \sigma^2 C)^{-1}A^Tb,$$

which has been derived in [13, Theorem 2.1]. Moreover, the result in Theorem 2.1 reduces to the result in [6, Theorem 2.1] when $\lambda = 1$.

Let $\tilde{A} = \begin{bmatrix} \tilde{A}_1 & \tilde{A}_2 \end{bmatrix} = A + \Delta A$ and $\tilde{b} = b + \Delta b$, where ΔA and Δb are perturbations of the input data A and b, respectively. Consider the perturbed MLSSTLS problem

$$\min_{E_2, f} \left\| \begin{bmatrix} E_2 & f \end{bmatrix} \right\|_F, \qquad \text{subject to} \quad \tilde{A}_1x_1 + (\tilde{A}_2 + E_2)\lambda x_2 = \lambda\tilde{b} + f. \tag{2.5}$$

When the norm $\left\| \begin{bmatrix} \Delta A & \lambda\Delta b \end{bmatrix} \right\|_F$ of the perturbations is sufficiently small, a perturbation analysis of the singular values can ensure that the perturbed MLSSTLS problem (2.5) has a unique solution $\tilde{x}_{\text{MS}}$. Let the change in the MLSSTLS solution be $\Delta x = \tilde{x}_{\text{MS}} - x_{\text{MS}}$. In [13, Theorem 3.7 and Lemma 3.8], the authors obtained the following first-order expression for Δx:

$$\begin{aligned}\Delta x &= \begin{bmatrix}-(DK)\otimes r^T - (D^{-1}x_{\text{MS}})^T \otimes B_\lambda & \frac{1}{\lambda}B_\lambda\end{bmatrix} \operatorname{vec}\left(\begin{bmatrix}\Delta A & \lambda\Delta b\end{bmatrix}\right)\\ &\quad + \mathcal{O}\left(\left\|\begin{bmatrix}\Delta A & \lambda\Delta b\end{bmatrix}\right\|_F^2\right),\end{aligned}$$

where

$$\begin{aligned}K &= (A^TA - \sigma^2 C)^{-1}, \qquad r = AD^{-1}x_{\text{MS}} - b, \qquad \text{and}\\ B_\lambda &= DK\left(A^T - \frac{2\lambda^2}{1+\|\lambda C x_{\text{MS}}\|_2^2} C x_{\text{MS}} r^T\right).\end{aligned}$$

The following theorem presents a new first-order expression for Δx:

THEOREM 2.3. *Let $H_0 = I_m - \frac{2rr^T}{\|r\|_2^2}$ and $G(x_{\text{MS}}) = \begin{bmatrix}(D^{-1}x_{\text{MS}})^T & -\frac{1}{\lambda}\end{bmatrix} \otimes I_m$. If $\left\|\begin{bmatrix}\Delta A & \lambda\Delta b\end{bmatrix}\right\|_F$ is sufficiently small, then*

$$\begin{aligned}\Delta x &= -DK\left(A^T H_0 G(x_{\text{MS}}) + \begin{bmatrix}I_n \otimes r^T & 0\end{bmatrix}\right) \operatorname{vec}\left(\begin{bmatrix}\Delta A & \lambda\Delta b\end{bmatrix}\right)\\ &\quad + \mathcal{O}\left(\left\|\begin{bmatrix}\Delta A & \lambda\Delta b\end{bmatrix}\right\|_F^2\right).\end{aligned}$$

Proof. To prove this theorem we only need to show that

$$\begin{bmatrix}-(DK)\otimes r^T - (D^{-1}x_{\text{MS}})^T \otimes B_\lambda & \frac{1}{\lambda}B_\lambda\end{bmatrix} = -DK\left(A^T H_0 G(x_{\text{MS}}) + \begin{bmatrix}I_n \otimes r^T & 0\end{bmatrix}\right).$$

It follows from Theorem 2.1 that

$$\begin{bmatrix}D^{-1}x_{\text{MS}}\\ -1\end{bmatrix}^T \begin{bmatrix}A^TA & A^Tb\\ b^TA & b^Tb\end{bmatrix} \begin{bmatrix}D^{-1}x_{\text{MS}}\\ -1\end{bmatrix} = \sigma^2 \begin{bmatrix}D^{-1}x_{\text{MS}}\\ -1\end{bmatrix}^T \begin{bmatrix}C & 0\\ 0 & \frac{1}{\lambda^2}\end{bmatrix} \begin{bmatrix}D^{-1}x_{\text{MS}}\\ -1\end{bmatrix},$$

i.e., $\sigma^2 = \frac{\|r\|_2^2}{\lambda^{-2}+\|Cx_{\text{MS}}\|_2^2}$. Since $x_{\text{MS}} = D(A^TA - \sigma^2 C)^{-1}A^Tb$ and $r = AD^{-1}x_{\text{MS}} - b$, we have

$$A^Tr = \sigma^2 C x_{\text{MS}} = \frac{\|r\|_2^2}{\lambda^{-2}+\|Cx_{\text{MS}}\|_2^2} C x_{\text{MS}}. \tag{2.6}$$

Consequently, we get

$$\begin{aligned}B_\lambda &= DK\left(A^T - \frac{2\lambda^2}{1+\|\lambda C x_{\text{MS}}\|_2^2} C x_{\text{MS}} r^T\right)\\ &= DK\left(A^T - \frac{2\lambda^2}{1+\|\lambda C x_{\text{MS}}\|_2^2} \frac{\lambda^{-2}+\|Cx_{\text{MS}}\|_2^2}{\|r\|_2^2} A^T r r^T\right)\\ &= DKA^TH_0.\end{aligned}$$

Note that for any $n\times m$ matrix M_1,

$$\begin{aligned}M_1 G(x_{\text{MS}}) &= M_1\left(\begin{bmatrix}(D^{-1}x_{\text{MS}})^T & -\frac{1}{\lambda}\end{bmatrix}\otimes I_m\right)\\ &= M_1\begin{bmatrix}\frac{1}{\lambda}x_{\text{MS}}^{(1)} I_m & \cdots & \frac{1}{\lambda}x_{\text{MS}}^{(n_1)} I_m & x_{\text{MS}}^{(n_1+1)} I_m & \cdots & x_{\text{MS}}^{(n)} I_m & -\frac{1}{\lambda}I_m\end{bmatrix}\\ &= \begin{bmatrix}\frac{1}{\lambda}x_{\text{MS}}^{(1)} M_1 & \cdots & \frac{1}{\lambda}x_{\text{MS}}^{(n_1)} M_1 & x_{\text{MS}}^{(n_1+1)} M_1 & \cdots & x_{\text{MS}}^{(n)} M_1 & -\frac{1}{\lambda}M_1\end{bmatrix}\\ &= \begin{bmatrix}(D^{-1}x_{\text{MS}})^T \otimes M_1 & -\frac{1}{\lambda}M_1\end{bmatrix}.\end{aligned}$$

Therefore, we have

$$\begin{aligned}
&\begin{bmatrix}-(DK)\otimes r^T-(D^{-1}x_{\text{MS}})^T\otimes B_\lambda & \frac{1}{\lambda}B_\lambda\end{bmatrix}\\
&\quad=\begin{bmatrix}-(D^{-1}x_{\text{MS}})^T\otimes B_\lambda & \frac{1}{\lambda}B_\lambda\end{bmatrix}+\begin{bmatrix}-(DK)\otimes r^T & 0\end{bmatrix}\\
&\quad=-DKA^TH_0G(x_{\text{MS}})-DK\begin{bmatrix}I_n\otimes r^T & 0\end{bmatrix}\\
&\quad=-DK\left(A^TH_0G(x_{\text{MS}})+\begin{bmatrix}I_n\otimes r^T & 0\end{bmatrix}\right).
\end{aligned}$$

We have thus proved the theorem. $\square$

According to Theorem 2.3 and the following two equalities

$$\begin{aligned}
G(x_{\text{MS}})\operatorname{vec}\left(\begin{bmatrix}\Delta A & \lambda\Delta b\end{bmatrix}\right)&=\left(\begin{bmatrix}(D^{-1}x_{\text{MS}})^T & -\frac{1}{\lambda}\end{bmatrix}\otimes I_m\right)\operatorname{vec}\left(\begin{bmatrix}\Delta A & \lambda\Delta b\end{bmatrix}\right)\\
&=\begin{bmatrix}(D^{-1}x_{\text{MS}})^T\otimes I_m & -\frac{1}{\lambda}I_m\end{bmatrix}\begin{bmatrix}\operatorname{vec}(\Delta A)\\ \lambda\Delta b\end{bmatrix}\\
&=\Delta AD^{-1}x_{\text{MS}}-\Delta b
\end{aligned}$$

and

$$\begin{bmatrix}I_n\otimes r^T & 0\end{bmatrix}\operatorname{vec}\left(\begin{bmatrix}\Delta A & \lambda\Delta b\end{bmatrix}\right)=\begin{bmatrix}I_n\otimes r^T & 0\end{bmatrix}\begin{bmatrix}\operatorname{vec}(\Delta A)\\ \lambda\Delta b\end{bmatrix}=\Delta A^Tr,$$

we can easily get that

$$\frac{\|\Delta x\|_2}{\|x_{\text{MS}}\|_2}\lesssim\left(\frac{\|DKA^T\|_2\|A\|_2}{\lambda}+\frac{\|DK\|_2\|r\|_2\|A\|_2}{\|x_{\text{MS}}\|_2}\right)\frac{\|\Delta A\|_2}{\|A\|_2}+\frac{\|DKA^T\|_2\|b\|_2}{\|x_{\text{MS}}\|_2}\frac{\|\Delta b\|_2}{\|b\|_2},$$

which can be found in [13, Theorem 5.1], but our proof is much simpler than the proofs there.

3. Condition numbers for the MLSSTLS problem. According to Theorem 2.3 and the concepts of the relative normwise condition number $\kappa^{\text{rel}}_{\text{MLSSTLS}}$, the mixed condition number $\kappa^{\text{mix}}_{\text{MLSSTLS}}$ and the componentwise condition number $\kappa^{\text{com}}_{\text{MLSSTLS}}$ for the MLSSTLS problem in [13], we can easily obtain the following theorem:

THEOREM 3.1. *Using the notation above, we have*

$$\kappa^{\text{rel}}_{\text{MLSSTLS}}=\frac{\left\|DK\left(A^TH_0G(x_{\text{MS}})+\begin{bmatrix}I_n\otimes r^T & 0\end{bmatrix}\right)\right\|_2\left\|\begin{bmatrix}A & \lambda b\end{bmatrix}\right\|_F}{\|x_{\text{MS}}\|_2},\tag{3.1}$$

$$\kappa^{\text{mix}}_{\text{MLSSTLS}}=\frac{\left\|\left|DK\left(A^TH_0G(x_{\text{MS}})+\begin{bmatrix}I_n\otimes r^T & 0\end{bmatrix}\right)\right|\operatorname{vec}\left(\begin{bmatrix}|A| & \lambda|b|\end{bmatrix}\right)\right\|_\infty}{\|x_{\text{MS}}\|_\infty},\tag{3.2}$$

and

$$\kappa^{\text{com}}_{\text{MLSSTLS}}=\left\|\frac{\left|DK\left(A^TH_0G(x_{\text{MS}})+\begin{bmatrix}I_n\otimes r^T & 0\end{bmatrix}\right)\right|\operatorname{vec}\left(\begin{bmatrix}|A| & \lambda|b|\end{bmatrix}\right)}{x_{\text{MS}}}\right\|_\infty.\tag{3.3}$$

REMARK 3.2. In [13, Theorem 4.2 and Theorem 4.4], the authors obtained

$$\begin{aligned}
\kappa^{\text{rel}}_{\text{MLSSTLS}}&=\frac{\|M+N\|_2\left\|\begin{bmatrix}A & \lambda b\end{bmatrix}\right\|_F}{\|x_{\text{MS}}\|_2},\\
\kappa^{\text{mix}}_{\text{MLSSTLS}}&=\frac{\left\||M+N|\operatorname{vec}\left(\begin{bmatrix}|A| & \lambda|b|\end{bmatrix}\right)\right\|_\infty}{\|x_{\text{MS}}\|_\infty}
\end{aligned}$$

and

$$\kappa_{\mathrm{MLSSTLS}}^{\mathrm{com}} = \left\| \frac{|M+N| \operatorname{vec}\left(\begin{bmatrix} |A| & \lambda|b| \end{bmatrix}\right)}{x_{\mathrm{MS}}} \right\|_\infty$$

with

$$\begin{aligned} M &= \begin{bmatrix} -(DK)\otimes r^T - (D^{-1}x_{\mathrm{MS}})^T \otimes (DKA^T) & \frac{1}{\lambda}DKA^T \end{bmatrix}, \\ N &= 2\sigma DKCx_{\mathrm{MS}} \begin{bmatrix} N_1 & N_2 \end{bmatrix}, \\ N_1 &= -\left(A_1^\dagger \begin{bmatrix} A_2 & \lambda b \end{bmatrix} v\right)^T \otimes u^T, \\ N_2 &= v^T \otimes u^T, \end{aligned}$$

and u, v being the left and right singular vectors of $P_{A_1}^\perp \begin{bmatrix} A_2 & \lambda b \end{bmatrix}$ corresponding to σ, respectively. Note that the orders of the matrices $DK\left(A^T H_0 G(x_{\mathrm{MS}}) + \begin{bmatrix} I_n \otimes r^T & 0 \end{bmatrix}\right)$ and $M+N$ are both $n \times (mn+m)$. Moreover, the matrices D, K, A and the vectors x_{MS}, r in $DK\left(A^T H_0 G(x_{\mathrm{MS}}) + \begin{bmatrix} I_n \otimes r^T & 0 \end{bmatrix}\right)$ are all used in M. It is distinctive that, unlike for the above three formulas, our formulas in Theorem 3.1 do not use the Moore-Penrose inverse $A_1^\dagger$ of A_1, and u and v. In addition, (3.1) reduces to the compact formula for the relative normwise condition number of the MTLS problem [7, Eq.(3.1)] in the case that $\lambda = 1$. When $n_1 = 0$ and $\lambda = 1$, (3.1) reduces to the compact formula for the relative normwise condition number of the TLS problem [4, Theorem 2].

The formula for the relative normwise condition numbers in Theorem 3.1 involves Kronecker products, which might lead to expensive storage and computational costs. In order to simply the relative normwise condition number of the MLSSTLS problem, we present the following theorem:

THEOREM 3.3. *If we partition the vector $x_{\mathrm{MS}} = \begin{bmatrix} x_{\mathrm{MS1}}^T & x_{\mathrm{MS2}}^T \end{bmatrix}^T$ with $x_{\mathrm{MS1}} \in \mathbb{R}^{n_1}$ and $x_{\mathrm{MS2}} \in \mathbb{R}^{n_2}$, then the relative normwise condition number of the MLSSTLS problem has the following equivalent forms:*

$$\kappa_{\mathrm{MLSSTLS}}^{\mathrm{rel}} = \frac{\left\| DK\left(\alpha A^T A - A^T r (D^{-1}x_{\mathrm{MS}})^T - D^{-1}x_{\mathrm{MS}} r^T A + \|r\|_2^2 I_n\right) KD \right\|_2^{1/2} \left\| \begin{bmatrix} A & \lambda b \end{bmatrix} \right\|_F}{\|x_{\mathrm{MS}}\|_2} \tag{3.4}$$

and

$$\kappa_{\mathrm{MLSSTLS}}^{\mathrm{rel}} = \frac{\left\| DK\left(\alpha A^T A + \begin{bmatrix} \|r\|_2^2 I_{n_1} & -\frac{\sigma^2}{\lambda} x_{\mathrm{MS1}} x_{\mathrm{MS2}}^T \\ -\frac{\sigma^2}{\lambda} x_{\mathrm{MS2}} x_{\mathrm{MS1}}^T & \|r\|_2^2 I_{n_2} - 2\sigma^2 x_{\mathrm{MS2}} x_{\mathrm{MS2}}^T \end{bmatrix}\right) KD \right\|_2^{1/2} \left\| \begin{bmatrix} A & \lambda b \end{bmatrix} \right\|_F}{\|x_{\mathrm{MS}}\|_2}, \tag{3.5}$$

where $\alpha = \frac{1}{\lambda^2} + \|D^{-1}x_{\mathrm{MS}}\|_2^2$.

Proof. By the properties of Kronecker product, we get

$$\begin{aligned} G(x_{\mathrm{MS}}) G(x_{\mathrm{MS}})^T &= \left(\frac{1}{\lambda^2} + \|D^{-1}x_{\mathrm{MS}}\|_2^2\right) I_m, \\ \begin{bmatrix} I_n \otimes r^T & 0 \end{bmatrix} (G(x_{\mathrm{MS}}))^T &= D^{-1} x_{\mathrm{MS}} r^T \end{aligned}$$

and

$$\begin{bmatrix} I_n \otimes r^T & 0 \end{bmatrix} \begin{bmatrix} I_n \otimes r^T & 0 \end{bmatrix}^T = \|r\|_2^2 I_n.$$

Thus, we have

$$\begin{aligned} DK &\left(A^T H_0 G(x_{\text{MS}}) + \begin{bmatrix} I_n \otimes r^T & 0 \end{bmatrix}\right) \left(A^T H_0 G(x_{\text{MS}}) + \begin{bmatrix} I_n \otimes r^T & 0 \end{bmatrix}\right)^T (DK)^T \\ &= DK \left(\alpha A^T A - A^T r (D^{-1} x_{\text{MS}})^T - D^{-1} x_{\text{MS}} r^T A + \|r\|_2^2 I_n\right) KD. \end{aligned} \tag{3.6}$$

The theorem follows immediately from Theorem 3.1, (2.6), (3.6), and the fact that for any real matrix L it holds that $\|L\|_2 = \|LL^T\|_2^{1/2}$ $\square$

REMARK 3.4. In (3.1), the matrix $DK\left(A^T H_0 G(x_{\text{MS}}) + \begin{bmatrix} I_n \otimes r^T & 0 \end{bmatrix}\right)$ is of size $n \times (mn+m)$, while the associated matrices in (3.4) and (3.5) are both of size $n \times n$, which is more economical with respect to storage. From the aspect of computation efficiency, the advantage of (3.5) over (3.4) is obvious since it requires less matrix-product operations.

In many applications, an upper bound would be sufficient to give an estimate of the conditioning of the MLSSTLS solution. According to (3.4) and (2.6), we can easily get the following theorem:

THEOREM 3.5. *Using the notation above, we have*

$$\begin{aligned} \kappa_{\text{MLSSTLS}}^{\text{rel}} \leq &\sqrt{\frac{\sigma^2 + \|A\|_2^2}{\lambda^2} + \|A\|_2^2 \|D^{-1} x_{\text{MS}}\|_2^2 + \sigma^2 \|C x_{\text{MS}}\|_2^2 + 2\sigma^2 \|D^{-1} x_{\text{MS}}\|_2 \|C x_{\text{MS}}\|_2} \\ &\times \frac{\|DK\|_2 \left\|\begin{bmatrix} A & \lambda b \end{bmatrix}\right\|_F}{\|x_{\text{MS}}\|_2}. \end{aligned}$$

In [13, Theorem 4.3], the authors obtained

$$\kappa_{\text{MLSSTLS}}^{\text{rel}} \leq \sqrt{\frac{\sigma^2 + \|A\|_2^2}{\lambda^2} + (3\sigma^2 + \|A\|_2^2) \|D^{-1} x_{\text{MS}}\|_2^2}\, \frac{\|DK\|_2 \left\|\begin{bmatrix} A & \lambda b \end{bmatrix}\right\|_F}{\|x_{\text{MS}}\|_2}. \tag{3.7}$$

Recalling that $C = \text{diag}(0_{n_1}, I_{n_2})$ and $D = \text{diag}(\lambda I_{n_1}, I_{n_2})$, we have

$$\|C x_{\text{MS}}\|_2 = \|C D^{-1} x_{\text{MS}}\|_2 \leq \|D^{-1} x_{\text{MS}}\|_2.$$

Hence the bound in Theorem 3.5 is always sharper than the one in (3.7).

4. Numercial experiments.

In [13], the authors obtained

$$\kappa_{\text{MLSSTLS}}^{\text{rel}} = \frac{\|M + N\|_2 \left\|\begin{bmatrix} A & \lambda b \end{bmatrix}\right\|_F}{\|x_{\text{MS}}\|_2}$$

and

$$M + N = \begin{bmatrix} -(DK) \otimes r^T - (D^{-1} x_{\text{MS}})^T \otimes B_\lambda & \frac{1}{\lambda} B_\lambda \end{bmatrix},$$

where

$$\begin{aligned} B_\lambda &= DK\left(A^T - \frac{2\lambda^2}{1 + \|\lambda C x_{\text{MS}}\|_2^2} C x_{\text{MS}} r^T\right), \\ M &= \begin{bmatrix} -(DK) \otimes r^T - (D^{-1} x_{\text{MS}})^T \otimes (DKA^T) & \frac{1}{\lambda} DKA^T \end{bmatrix}, \\ N &= 2\sigma DKC x_{\text{MS}} \begin{bmatrix} N_1 & N_2 \end{bmatrix}, \\ N_1 &= -\left(A_1^\dagger \begin{bmatrix} A_2 & \lambda b \end{bmatrix} v\right)^T \otimes u^T, \qquad N_2 = v^T \otimes u^T \end{aligned}$$

and u, and v are the left and right singular vectors of $P_{A_1}^{\perp}\begin{bmatrix}A_2 & \lambda b\end{bmatrix}$ corresponding to σ, respectively. Consequently, we can get

$$\kappa_{\mathrm{MLSSTLS}}^{\mathrm{rel}} = \frac{\left\|\begin{bmatrix}-(DK)\otimes r^T-(D^{-1}x_{\mathrm{MS}})^T\otimes B_\lambda & \frac{1}{\lambda}B_\lambda\end{bmatrix}\right\|_2 \left\|\begin{bmatrix}A & \lambda b\end{bmatrix}\right\|_F}{\|x_{\mathrm{MS}}\|_2}. \tag{4.1}$$

In this section, we report numerical experiments to illustrate that the CPU times using (3.4) and (3.5) for computing the relative normwise condition number are smaller than when using (3.1) and (4.1). All the numerical experiments were performed using MATLAB R2016a with machine precision 2.2204×10^{-16}.

EXAMPLE 4.1. [13] Consider the MLSSTLS problem (1.2), and let

$$\begin{bmatrix}A & b\end{bmatrix} = Q\begin{bmatrix}A_{11} & A_{12} & A_{1b}\\ 0 & A_{22} & A_{2b}\end{bmatrix} \in \mathbb{R}^{m\times(n+1)},$$

where $Q = I_m - 2yy^T$ with $y \in \mathbb{R}^m$ being a random unit vector,

$$\begin{aligned} A_{11} &= c \times \mathrm{eye}(20) + \mathrm{triu}(\mathrm{rand}(20)), \qquad \text{with } c > 0,\\ A_{12} &= \mathrm{rand}(20, n-20), \qquad A_{1b} = \mathrm{ones}(20,1),\\ A_{22} &= \mathrm{diag}((n-20):-1:1) \in \mathbb{R}^{(m-20)\times(n-20)}, \text{ and}\\ A_{2b} &= \begin{bmatrix}\mathrm{ones}(1,n-19) & \mathrm{zeros}(1,m-n-1)\end{bmatrix}^T. \end{aligned}$$

In the experiment, we set $c = 0.8, m = 600, n = 120, n_1 = 100$. We report the computed results (denoted by CR) and the elapsed CPU times in seconds (denoted by CPU) for computing the relative normwise condition number $\kappa_{\mathrm{MLSSTLS}}^{\mathrm{rel}}$ by using formulas (3.1), (3.4), (3.5), and (4.1) for various values of λ in Table 4.1 We can see from Table 4.1 that the computed results are always equal for the different formulas but the elapsed CPU times using (3.4) and (3.5) are much smaller than those for (3.1) and (4.1).

TABLE 4.1
Computed results and CPU times for the computation of $\kappa_{\mathrm{MLSSTLS}}^{\mathrm{rel}}$.

		λ=1e-05	λ=5	λ=1e+05
(3.1)	CR	4.6092e+07	4.1959e+03	1.7876e+07
	CPU	1.4350	1.4366	1.4227
(3.4)	CR	4.6092e+07	4.1959e+03	1.7876e+07
	CPU	0.0075	0.0071	0.0065
(3.5)	CR	4.6092e+07	4.1959e+03	1.7876e+07
	CPU	0.0044	0.0046	0.0054
(4.1)	CR	4.6092e+07	4.1959e+03	1.7876e+07
	CPU	1.1077	1.1492	1.1410

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