



ON CONDITION NUMBERS OF QUATERNION MATRIX INVERSE AND QUATERNION LINEAR SYSTEMS WITH MULTIPLE RIGHT-HAND SIDES*

QIAOHUA LIU[†], SHAN WANG[†], AND FENGXIA ZHANG[‡]

Abstract. This paper is devoted to the condition numbers of quaternion linear system with multiple right-hand sides and the associated condition numbers of the quaternion matrix inverse as well. The explicit expressions of the unstructured and structured normwise, mixed, and componentwise condition numbers for the system are given. To reduce the computational cost of the condition numbers, compact and tight upper bounds for these condition numbers are proposed. For general sparse and badly scaled problems, numerical examples show that mixed and componentwise condition numbers are preferred than the normwise condition number for estimating the forward error of the solution, and structured condition numbers are tighter than the unstructured ones for some specific structured problems.

Key words. Quaternion linear system, Multiple right-hand sides, Quaternion matrix inverse, Normwise condition number, Mixed condition number, Componentwise condition number, Structured condition number.

AMS subject classifications. 15A12, 65F35.

1. Introduction. Quaternions, invented by W. Hamilton in 1843 [10] and quaternion matrices [38], have been widely used in many research fields such as quaternionic quantum [5], group representations [30, 31], field theory [3], and image processing [14, 15, 16]. As a basic tool, the $n \times n$ nonsingular quaternion linear system

$$(1.1) \quad AX = B,$$

with t right-hand sides has attracted much attention, both in numerical computations and theoretical properties. For example, in the quaternion toolbox for MATLAB (QTFM) [29], Sangwine and Le Bihan developed quaternion LU on the basis of quaternion arithmetic operations. By exploring the real counterpart of a quaternion matrix, the authors in [21, 32] developed real structure-preserving LU algorithms to improve the efficiency of the computation. Liu et al., [24] studied the accuracy and stability of quaternion LU and quaternion Gaussian elimination. For further information on other quaternion matrix factorizations such as quaternion Cholesky, quaternion QR [23], and quaternion SVD [22, 23], we refer to [14, 15, 16, 17] and the monographs [13, 34] for more information on quaternion matrix computation problems.

It is of interest that when a numerical algorithm applied to (1.1) is backward stable, how close the numerical solution is to the exact solution. The condition number is a vital tool that measures the worst-case sensitivity of its solution to small perturbations in the input data. Combined with backward errors, it provides a (possibly approximate) upper bound for the forward error, i.e., the difference between a perturbed solution and the exact solution. The problem with a large condition number is called an *ill-posed* problem

*Received by the editors on March 1, 2023. Accepted for publication on August 31, 2023. Handling Editor: Heike Fassbender. Corresponding Author: Qiaohua Liu.

Funding: The work of the authors was partially supported by the Natural Science Foundation of Shanghai, China under grant 23ZR1422400 and the Natural Science Foundation of Shandong Province, China under grant ZR2022MA030.

[†]Department of Mathematics, Shanghai University, Shanghai 200444, P. R. China, and Newtown Center for Mathematics of Shanghai University, 99 Shangda Road, Shanghai 200444, P. R. China (qhliu@shu.edu.cn).

[‡]College of Mathematical Science, Liaocheng University, Liaocheng 252000, P.R. China (zhangfengxia@lcu.edu.cn).

[12]. This paper focuses on the condition numbers of quaternion linear system (1.1) and quaternion matrix inverse. How the perturbations affect the quaternion solution remains unknown. To our knowledge, no literature has specifically addressed this issue.

A frequently used tool in the real conditioning analysis is based on the concept of normwise condition number [6, 26], mixed, and componentwise condition numbers [2, 7]. Let $x = \phi(a)$ be a nonzero continuous and Fréchet differentiable mapping from \mathbb{R}^p to \mathbb{R}^q . Set $\delta x = \phi(a + \delta a) - \phi(a)$ and let $d\phi(a)$ be the Fréchet derivative of ϕ at a . The normwise, mixed, and componentwise condition number are defined and formulated as

$$\begin{aligned} \kappa(\phi, a) &:= \lim_{\varepsilon \rightarrow 0} \sup_{\|\delta a\|_2 \leq \varepsilon \|a\|_2} \frac{\|\delta x\|_2 / \|x\|_2}{\|\delta a\|_2 / \|a\|_2} = \frac{\|d\phi(a)\|_2 \|a\|_2}{\|\phi(a)\|_2}, \\ m(\phi, a) &:= \lim_{\varepsilon \rightarrow 0} \sup_{|\delta a| \leq \varepsilon |a|} \frac{\|\delta x\|_\infty / \|x\|_\infty}{\|\delta a/a\|_\infty} = \frac{\|d\phi(a)\|_\infty \|a\|_\infty}{\|\phi(a)\|_\infty}, \\ c(\phi, a) &:= \lim_{\varepsilon \rightarrow 0} \sup_{|\delta a| \leq \varepsilon |a|} \frac{\|\delta x/x\|_\infty}{\|\delta a/a\|_\infty} = \left\| \frac{d\phi(a)\|a\|}{|\phi(a)|} \right\|_\infty, \end{aligned}$$

where $|a|$ denotes a vector by taking the entrywise absolute value, b/a or $\frac{b}{a}$ is the entrywise division. Note that $\xi/0$ is interpreted as zero if $\xi = 0$ and infinity otherwise. In this paper, we only consider the case that $\|b/a\|_\infty$ is finite.

Based on the real condition number theory, condition numbers of the real matrix inverse and real linear system have been widely studied in the literature. We refer the reader to [2, 4, 9, 11, 12, 27, 28, 36]. For quaternion linear systems, these conditioning theories are not necessarily applicable. In order to establish the perturbation results of the quaternion system based on the existing condition number theory, in this paper, we transform (1.1) into a real linear system involving four Kronecker products by making use of the real counterpart of a quaternion matrix. Different from the work [1, 4, 19, 39, 35] for studying condition numbers of the real Kronecker product linear system such as $(C \otimes D)X = F$, the quaternion linear system (1.1) is equivalent to a real system like $\sum_{i=1}^4 (C_i \otimes D_i)X = F$. The condition numbers of such linear system with four Kronecker products are generally quite difficult to analyze. Fortunately, some matrices in the equivalent Kronecker product system of (1.1) take special forms and are not perturbed, which allows explicit expressions for the first order perturbation estimate of (1.1). Based on this observation, the normwise, mixed, and componentwise condition numbers are established, and the condition numbers of the inverse of nonsingular quaternion matrices can also derived by setting $B = I_n$ in (1.1) and restricting no perturbations on B .

Before our discussion, some notations are required. $\mathbb{R}^{m \times n}$ and $\mathbb{Q}^{m \times n}$ denote the spaces of $m \times n$ real and quaternion matrices, respectively. I_n denotes the $n \times n$ identity matrix. $O_{m \times n}$, O_n denote the $m \times n$, $n \times n$ zero matrices, respectively. $e_{n \times 1}$ denotes an $n \times 1$ vector of all ones. If subscripts are ignored, the sizes of identity and zero matrices are clear from the context. $\|\cdot\|_2$, $\|\cdot\|_\infty$ and $\|\cdot\|_F$ denote 2-norm, ∞ -norm and Frobenius norm of their arguments, respectively. For a real matrix A , $|A|$ is a matrix by taking the entrywise absolute value, $\|A\|_{\max}$ denotes the maximal absolute value of elements in A , A^T is the transpose of A . $\text{vec}(A)$ is an operator, which stacks the columns of A one underneath the other.

For matrices $A \in \mathbb{R}^{m \times n}$, $B \in \mathbb{R}^{p \times q}$, the Kronecker product [20] of A and B denoted by $A \otimes B = [a_{ij}B]$ has the following properties [8, 20]:

$$(1.2) \quad |A \otimes B| = |A| \otimes |B|, \quad \|(A \otimes B)\|_2 = \|A\|_2 \|B\|_2,$$

$$(1.3) \quad (A \otimes B) \otimes C = A \otimes (B \otimes C),$$

$$(1.4) \quad (A \otimes C)(B \otimes D) = (AB) \otimes (CD),$$

$$(1.5) \quad (A \otimes B)^T = A^T \otimes B^T,$$

$$(1.6) \quad \text{vec}(AXB) = (B^T \otimes A)\text{vec}(X),$$

$$(1.7) \quad \text{vec}(A \otimes B) = (I_n \otimes \Pi_{q,m} \otimes I_p)[\text{vec}(A) \otimes \text{vec}(B)],$$

where $\Pi_{q,m}$ is a $qm \times qm$ permutation matrix such that $\text{vec}(C^T) = \Pi_{q,m}\text{vec}(C)$ for any $C \in \mathbb{R}^{q \times m}$.

2. Preliminaries. In this section, we first introduce some basic information for quaternion matrices. A quaternion $q \in \mathbb{Q}$ has one real part and three imaginary parts as

$$q = q_1 + q_2i + q_3j + q_4k,$$

where $q_1, q_2, q_3, q_4 \in \mathbb{R}$, and i, j and k are three imaginary units satisfying

$$i^2 = j^2 = k^2 = -1, \quad ij = -ji = k, \quad jk = -kj = i, \quad ki = -ik = j.$$

Note that quaternion skew-field \mathbb{Q} is an associative but noncommutative algebra of rank four over \mathbb{R} . The conjugate, modulus of q are defined by

$$q^* = q_1 - q_2i - q_3j - q_4k, \quad \|q\| = \sqrt{q_1^2 + q_2^2 + q_3^2 + q_4^2},$$

and the inverse of q is given by $q^{-1} = q^*/\|q\|^2$ provided that $\|q\| \neq 0$.

For any quaternion matrices $P = P_1 + P_2i + P_3j + P_4k \in \mathbb{Q}^{m \times n}$, $Q = Q_1 + Q_2i + Q_3j + Q_4k \in \mathbb{Q}^{m \times n}$, the conjugate of Q is given by $Q^* = Q_1^T - Q_2^T i - Q_3^T j - Q_4^T k$, and the sum of P, Q is

$$P + Q = (P_1 + Q_1) + (P_2 + Q_2)i + (P_3 + Q_3)j + (P_4 + Q_4)k.$$

For the quaternion matrix $S \in \mathbb{Q}^{n \times \ell}$, the multiplication QS is given by

$$\begin{aligned} & (Q_1S_1 - Q_2S_2 - Q_3S_3 - Q_4S_4) + (Q_1S_2 + Q_2S_1 + Q_3S_4 - Q_4S_3)i + \\ & (Q_1S_3 - Q_2S_4 + Q_3S_1 + Q_4S_2)j + (Q_1S_4 + Q_2S_3 - Q_3S_2 + Q_4S_1)k. \end{aligned}$$

Let

$$(2.8) \quad \Upsilon_Q = \begin{bmatrix} Q_1 & -Q_2 & -Q_3 & -Q_4 \\ Q_2 & Q_1 & -Q_4 & Q_3 \\ Q_3 & Q_4 & Q_1 & -Q_2 \\ Q_4 & -Q_3 & Q_2 & Q_1 \end{bmatrix} \in \mathbb{R}^{4m \times 4n},$$

be a linear homeomorphic mapping from the quaternion matrix $Q \in \mathbb{Q}^{m \times n}$ to its real counterpart. Even though there are many different real counterparts (see, e.g., [17, 23]), it is interesting to note that they are permutation equivalent (see [18, Remark 4.7]) and the real counterpart has the following properties [17, 23]:

$$(2.9) \quad \begin{aligned} i) & \quad \Upsilon_{k_1P+k_2Q} = k_1\Upsilon_P + k_2\Upsilon_Q, \quad k_1, k_2 \in \mathbb{R}; \\ ii) & \quad \Upsilon_{k_1Q^*} = k_1\Upsilon_Q^T, \quad \Upsilon_{QS} = \Upsilon_Q\Upsilon_S; \\ iii) & \quad \Upsilon_{Q^{-1}} = (\Upsilon_Q)^{-1} \text{ if } Q \text{ is invertible}; \\ iv) & \quad 2\|Q\|_F = \|\Upsilon_Q\|_F, \quad \|Q\|_2 = \|\Upsilon_Q\|_2. \end{aligned}$$

This means the real algebraic symmetry structure of Υ_Q is preserved under above arithmetic operations. We use

$$Q_r = [Q_1 \ Q_2 \ Q_3 \ Q_4], \quad Q_c = [Q_1^T \ Q_2^T \ Q_3^T \ Q_4^T]^T,$$

to denote the row and column representations of Q . In the latter analysis, we also use $\text{col}(Q_r)$ instead of Q_c to stack the block columns of Q_r one underneath another.

For the quaternion linear system (1.1) with t right-hand sides, write $A = A_1 + A_2i + A_3j + A_4k$. Let $\tilde{A}_i = A_i + \Delta A_i, \tilde{B}_i = B_i + \Delta B_i$, where ΔA_i and ΔB_i denote the perturbations to the four parts of A and B , respectively. For the data space $\mathbb{R}^{n \times 4n} \times \mathbb{R}^{n \times 4t}$, we use the weighted norm

$$\|[\Delta A_r \ \Delta B_r]\|_{\mathcal{F}} = \sqrt{\|\Delta A_r^\alpha\|_F^2 + \|\Delta B_r^\beta\|_F^2},$$

where

$$\Delta A_r^\alpha = [\alpha_1 \Delta A_1 \ \alpha_2 \Delta A_2 \ \alpha_3 \Delta A_3 \ \alpha_4 \Delta A_4], \quad \Delta B_r^\beta = [\beta_1 \Delta B_1 \ \beta_2 \Delta B_2 \ \beta_3 \Delta B_3 \ \beta_4 \Delta B_4].$$

Here the positive numbers α_i and β_i ($i = 1, \dots, 4$) are designed to monitor the perturbations on A_i and B_i in the flexible norms. For instance, when α_1 tends to infinity, it enables to obtain condition number problems where A_1 is not perturbed. The idea of using parameters to unify the perturbations and conditions was first proposed in [9] and then used or extended in [33, 37].

Due to the difficulties in dealing with the perturbation analysis for four parts of ΔX , we use (2.9) to transform (1.1) into the real linear system $\Upsilon_A \Upsilon_X = \Upsilon_B$. Since Υ_X has the special algebraic symmetry structure, we only consider its first block column, i.e.,

$$(2.10) \quad \Upsilon_A X_c = B_c,$$

and define the mapping $\phi : \mathbb{R}^{4n^2+4nt} \mapsto \mathbb{R}^{kt}$ with

$$\phi(a) := \text{vec}(L^T \Upsilon_A^{-1} B_c) \quad \text{for} \quad a := \begin{bmatrix} \text{vec}(A_r) \\ \text{vec}(B_c) \end{bmatrix},$$

where L is a $4n$ -by- k ($k \leq 4n$) matrix introduced for the selection of the solution components. For example, when $L^T = I_{4n}$, all the $4n$ rows of the solution X_c are equally selected. When $L^T = e_i^T$, i.e., the i th row of I_{4n} , only the i th row of the solution is selected. We can also choose appropriate L^T to select rows of X_c corresponding to real/imaginary parts in the quaternion solution.

For the quaternion linear system (1.1), the normwise condition number $\kappa(L, A_r, B_r)$, the mixed condition number $m(L, A_r, B_r)$, and the componentwise condition number $c(L, A_r, B_r)$ are defined as follows.

DEFINITION 2.1.

$$(2.11) \quad \kappa(L, A_r, B_r) = \lim_{\epsilon \rightarrow 0} \sup_{\|[\Delta A_r \ \Delta B_r]\|_{\mathcal{F}} \leq \epsilon \| [A_r \ B_r] \|_{\mathcal{F}}} \frac{\|L^T \Delta X_c\|_F}{\epsilon \|L^T X_c\|_F},$$

$$(2.12) \quad m(L, A_r, B_r) = \lim_{\epsilon \rightarrow 0} \sup_{|\Delta A_r \ \Delta B_r| \leq \epsilon |A_r \ B_r|} \frac{\|L^T \Delta X_c\|_{\max}}{\epsilon \|L^T X_c\|_{\max}},$$

$$(2.13) \quad c(L, A_r, B_r) = \lim_{\epsilon \rightarrow 0} \sup_{|\Delta A_r \ \Delta B_r| \leq \epsilon |A_r \ B_r|} \frac{1}{\epsilon} \left\| \frac{L^T \Delta X_c}{|L^T X_c|} \right\|_{\max}.$$

According to the concept of condition numbers in Section 1, it is obvious that

$$m(L, A_r, B_r) = \frac{\|d\phi(a)\|_a}{\|\phi(a)\|_\infty}, \quad c(L, A_r, B_r) = \left\| \frac{d\phi(a)\|a\|}{|\phi(a)|} \right\|_\infty.$$

As for the formula for the flexible normwise condition number $\kappa(L, A_r, B_r)$, we need to define the mapping $\bar{\phi}$ as

$$\text{vec}(L^T X_c) = \bar{\phi}(\bar{a}) \quad \text{with} \quad \bar{a} := \begin{bmatrix} \text{vec}(A_r^\alpha) \\ \text{vec}(B_c^\beta) \end{bmatrix},$$

where $B_c^\beta = \text{col}(B_r^\beta)$. The normwise condition number is then formulated as

$$\kappa(L, A_r, B_r) = \frac{\|d\bar{\phi}(\bar{a})\|_2 \|\bar{a}\|_2}{\|\bar{\phi}(\bar{a})\|_2}.$$

If we take $B_r = [I_n \ O_n \ O_n \ O_n]$ and ΔB_r to be a zero matrix in the definition, we obtain the condition numbers of the quaternion matrix inverse A^{-1} .

3. Condition numbers for unstructured matrices. In this section, we evaluate the condition number of quaternion linear equation (1.1), where the quaternion matrices A, B are unstructured. Write Υ_A in (2.10) as

$$(3.14) \quad \Upsilon_A = S_1 \otimes A_1 + S_2 \otimes A_2 + S_3 \otimes A_3 + S_4 \otimes A_4,$$

where

$$(3.15) \quad S_1 = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}, S_2 = \begin{bmatrix} 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \end{bmatrix}, S_3 = \begin{bmatrix} 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{bmatrix}, S_4 = \begin{bmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix}.$$

The real linear system (2.10) now becomes

$$(3.16) \quad \sum_{i=1}^4 (S_i \otimes A_i) X_c = B_c,$$

and in the perturbed system, the matrices S_1, S_2, S_3, S_4 are not perturbed. For perturbations small enough, $\Upsilon_{A+\Delta A}$ is nonsingular, and the perturbed system takes the form

$$(3.17) \quad \sum_{i=1}^4 (S_i \otimes (A_i + \Delta A_i))(X_c + \Delta X_c) = B_c + \Delta B_c.$$

THEOREM 3.1. *With the notation in (3.14)–(3.17), let $s_i = \text{vec}(S_i)$ for $i = 1, 2, \dots, 4$ and set the 16-by-4 matrix $S = [s_1 \ s_2 \ s_3 \ s_4]$. For the Fréchet differential of the solution, we have*

$$\text{vec}(L^T dX_c) = K \begin{bmatrix} \text{vec}(dA_r) \\ \text{vec}(dB_c) \end{bmatrix},$$

where

$$(3.18) \quad K := d\phi \left(\begin{bmatrix} \text{vec}(A_r) \\ \text{vec}(B_c) \end{bmatrix} \right) = (I_t \otimes (L^T \Upsilon_A^{-1})) [-Q(S \otimes I_{n^2}) \quad I_{4nt}],$$

with $Q = (X_c^T \otimes I_{4n})(I_4 \otimes \Pi_{n,4} \otimes I_n)$.

Proof. We have the differential of the system (3.16) as

$$\sum_{i=1}^4 (S_i \otimes A_i)(dX_c) + \sum_{i=1}^4 (S_i \otimes dA_i)X_c = dB_c.$$

It follows that

$$(3.19) \quad L^T dX_c = L^T \Upsilon_A^{-1} (dB_c - \sum_{i=1}^4 (S_i \otimes dA_i)X_c).$$

Therefore, we obtain from the properties in (1.6)–(1.7) that

$$\begin{aligned} \text{vec}(L^T dX_c) &= (I_t \otimes (L^T \Upsilon_A^{-1})) \left(\text{vec}(dB_c) - \sum_{i=1}^4 (X_c^T \otimes I_{4n}) \text{vec}(S_i \otimes dA_i) \right) \\ &= (I_t \otimes (L^T \Upsilon_A^{-1})) \left(\text{vec}(dB_c) - (X_c^T \otimes I_{4n})(I_4 \otimes \Pi_{n,4} \otimes I_n) \sum_{i=1}^4 \text{vec}(S_i) \otimes \text{vec}(dA_i) \right) \\ &= (I_t \otimes (L^T \Upsilon_A^{-1})) \left(\text{vec}(dB_c) - Q \sum_{i=1}^4 (\text{vec}(S_i) \otimes I_{n^2}) \text{vec}(dA_i) \right) \\ (3.20) \quad &= (I_t \otimes (L^T \Upsilon_A^{-1})) \begin{bmatrix} -Q(S \otimes I_{n^2}) & I_{4nt} \end{bmatrix} \begin{bmatrix} \text{vec}(dA_r) \\ \text{vec}(dB_c) \end{bmatrix}. \end{aligned}$$

We derive that

$$d\phi \left(\begin{bmatrix} \text{vec}(A_r) \\ \text{vec}(B_c) \end{bmatrix} \right) = (I_t \otimes (L^T \Upsilon_A^{-1})) \begin{bmatrix} -Q(S \otimes I_{n^2}) & I_{4nt} \end{bmatrix}.$$

This completes the proof. □

For positive numbers α_i and β_i , it should be noted that

$$(3.21) \quad \text{vec}(L^T dX_c) = \bar{K} \begin{bmatrix} \text{vec}(dA_r^\alpha) \\ \text{vec}(dB_c^\beta) \end{bmatrix},$$

where

$$(3.22) \quad \bar{K} = (I_t \otimes (L^T \Upsilon_A^{-1})) \begin{bmatrix} -Q(S_\alpha \otimes I_{n^2}) & T_\beta \end{bmatrix} \quad \text{with} \\ S_\alpha = [\alpha_1^{-1} s_1 \quad \alpha_2^{-1} s_2 \quad \alpha_3^{-1} s_3 \quad \alpha_4^{-1} s_4], \quad T_\beta = I_t \otimes \text{diag}(\beta_1^{-1} I_n, \beta_2^{-1} I_n, \beta_3^{-1} I_n, \beta_4^{-1} I_n).$$

By the concept of the normwise condition number defined in section 2, we derive the normwise condition number for (1.1) as below

$$(3.23) \quad \kappa(L, A_r, B_r) = \|\bar{K}\|_2 \frac{\|[A_r \ B_r]\|_{\mathcal{F}}}{\|L^T X_c\|_F}.$$

It is observed that the explicit expression in (3.23) involves the Kronecker product operations which might lead to large storage and computational cost. The following theorem gives the compact upper bound of the normwise condition number.

THEOREM 3.2. *With the notation of Theorem 3.1 and the expressions in (3.21)–(3.22), the normwise condition number given in (3.23) has the compact upper bound as*

$$(3.24) \quad \kappa^u(L, A_r, B_r) = \left(c_1 \|X_c\|_2^2 + c_2 \right)^{1/2} \|L^T \Upsilon_A^{-1}\|_2 \frac{\|[A_r \ B_r]\|_{\mathcal{F}}}{\|L^T X_c\|_F},$$

where $c_1 = \max_{1 \leq i \leq 4} \{4\alpha_i^{-2}\}$, $c_2 = \max_{1 \leq i \leq 4} \{\beta_i^{-2}\}$.

Proof. In (3.22), by setting $M = [-Q(S_\alpha \otimes I_{n^2}) \quad T_\beta]$, we obtain from (1.2) to (1.5) that

$$(3.25) \quad \begin{aligned} \|MM^T\|_2 &= \|Q(S_\alpha S_\alpha^T \otimes I_{n^2})Q^T + T_\beta T_\beta^T\|_2 \\ &\leq \|Q\|_2^2 \|(S_\alpha S_\alpha^T) \otimes I_{n^2}\|_2 + \|T_\beta T_\beta^T\|_2 \\ &= \|X_c\|_2^2 \|S_\alpha^T S_\alpha\|_2 + c_2 = c_1 \|X_c\|_2^2 + c_2, \end{aligned}$$

where we have used the facts that

$$\begin{aligned} \|Q\|_2^2 &= \|QQ^T\|_2 = \|(X_c^T X_c) \otimes I_{4n}\|_2 = \|X_c\|_2^2, \\ S_\alpha^T S_\alpha &= \text{diag}(4\alpha_1^{-2}, 4\alpha_2^{-2}, 4\alpha_3^{-2}, 4\alpha_4^{-2}). \end{aligned}$$

Consequently,

$$\begin{aligned} \|\bar{K}\bar{K}^T\|_2 &= \|(I_t \otimes (L^T \Upsilon_A^{-1}))MM^T(I_t \otimes (L^T \Upsilon_A^{-1}))^T\|_2 \\ &\leq \|(I_t \otimes (L^T \Upsilon_A^{-1}))\|_2^2 \|MM^T\|_2 \\ &\leq \|L^T \Upsilon_A^{-1}\|_2^2 (c_1 \|X_c\|_2^2 + c_2), \end{aligned}$$

from which we deduce that

$$\|\bar{K}\|_2 = \|\bar{K}\bar{K}^T\|_2^{1/2} \leq \|L^T \Upsilon_A^{-1}\|_2 (c_1 \|X_c\|_2^2 + c_2)^{1/2}.$$

This yields the estimate in (3.24). □

THEOREM 3.3. *With the notation of Theorem 3.1, let*

$$\mathcal{M} = -(I_t \otimes (L^T \Upsilon_A^{-1}))Q(S \otimes I_{n^2}), \quad \mathcal{N} = I_t \otimes (L^T \Upsilon_A^{-1}).$$

Then, the mixed and componentwise condition numbers of the quaternion linear system (1.1) have the following forms:

$$\begin{aligned} m(L, A_r, B_r) &= \frac{\|\mathcal{M}\|\text{vec}(|A_r|) + \|\mathcal{N}\|\text{vec}(|B_c|)}{\|L^T X_c\|_{\max}}, \\ c(L, A_r, B_r) &= \left\| \frac{\|\mathcal{M}\|\text{vec}(|A_r|) + \|\mathcal{N}\|\text{vec}(|B_c|)}{\text{vec}(L^T X_c)} \right\|_{\infty}. \end{aligned}$$

They have sharp bounds as

$$(3.26) \quad m(L, A_r, B_r) \leq \frac{\|L^T \Upsilon_A^{-1}(\Upsilon_{|A|_*} |X_c| + |B_c|)\|_{\max}}{\|L^T X_c\|_{\max}},$$

$$(3.27) \quad c(L, A_r, B_r) \leq \left\| \frac{L^T \Upsilon_A^{-1} \Upsilon_{|A|_*} |X_c| + L^T \Upsilon_A^{-1} |B_c|}{|L^T X_c|} \right\|_{\max},$$

where $\Upsilon_{|A|_*}$ is the real counterpart of $|A|_*$ with $|A|_*$ defined by $|A|_* = |A_1| + |A_2|i + |A_3|j + |A_4|k$.

Proof. From Theorem 3.1 and Definition 2.1, it is straightforward that

$$\begin{aligned}
 m(L, A_r, B_r) &= \frac{\left\| (I_t \otimes (L^T \Upsilon_A^{-1})) \begin{bmatrix} -Q(S \otimes I_{n^2}) & I_{4nt} \end{bmatrix} \begin{bmatrix} \text{vec}(|A_r|) \\ \text{vec}(|B_c|) \end{bmatrix} \right\|_{\infty}}{\|L^T X_c\|_{\max}} \\
 &\leq \frac{\left\| (I_t \otimes |L^T \Upsilon_A^{-1}|) |Q| \sum_{j=1}^4 (|\text{vec}(S_j)| \otimes I_{n^2}) \text{vec}(|A_j|) + (I_t \otimes (L^T \Upsilon_A^{-1})) |\text{vec}(|B_c|)| \right\|_{\infty}}{\|L^T X_c\|_{\max}} \\
 &= \frac{\left\| |L^T \Upsilon_A^{-1}| \sum_{j=1}^4 (|S_j| \otimes |A_j|) |X_c| + |L^T \Upsilon_A^{-1}| |B_c| \right\|_{\max}}{\|L^T X_c\|_{\max}},
 \end{aligned}$$

in which $\sum_{j=1}^4 (\text{vec}(|S_j|) \otimes |A_j|)$ is just the real counterpart of $|A|_*$. The above relations yield the formula and upper bound for the mixed condition number. The upper bound for $c(L, A_r, B_r)$ can be obtained in a similar way. \square

For the condition numbers of the quaternion matrix inverse, we denote $A^{-1} = \bar{A} = \bar{A}_1 + \bar{A}_2 i + \bar{A}_3 j + \bar{A}_4 k$, and rewrite (2.10) as $\Upsilon_A \bar{A}_c = B_c$ with $B_c = [I_n \ O_n \ O_n \ O_n]^T$. Note that B_c is not perturbed. Thus, the normwise condition number of \bar{A}_c can be obtained by letting $\beta_i \rightarrow \infty$ in (3.24) for $i = 1, 2, 3, 4$. The mixed and componentwise condition numbers can be derived by setting ΔB_c and dB_c to be zero in (3.17) and (3.20), from which we obtain $d\phi(\text{vec}(A_r)) = \mathcal{M}$ and the theorem as follows.

THEOREM 3.4. *Let c_1 , \mathcal{M} and $|A|_*$ be defined in Theorems 3.2 and 3.3. Set $\|A_r\|_f := \|[A_r \ O_{n \times 4n}]\|_{\mathcal{F}}$. Then, the condition numbers of $\bar{A} := A^{-1}$ are given as follows*

$$\begin{aligned}
 \kappa(L, A_r) &= \|\mathcal{M}\|_2 \frac{\|A_r\|_f}{\|L^T \bar{A}_c\|_2} \leq c_1^{1/2} \|\bar{A}_c\|_2 \|L^T \Upsilon_A^{-1}\|_2 \frac{\|A_r\|_f}{\|L^T \bar{A}_c\|_F}, \\
 m(L, A_r) &= \frac{\|\|\mathcal{M}|\text{vec}(|A_r|)\|_{\infty}\|}{\|L^T \bar{A}_c\|_{\max}} \leq \frac{\| |L^T \Upsilon_A^{-1}| \Upsilon_{|A|_*} |\bar{A}_c| \|_{\max}}{\|L^T \bar{A}_c\|_{\max}}, \\
 c(L, A_r) &= \left\| \frac{\|\mathcal{M}|\text{vec}(|A_r|)\|_{\infty}}{\text{vec}(L^T \bar{A}_c)} \right\|_{\infty} \leq \left\| \frac{|L^T \Upsilon_A^{-1}| \Upsilon_{|A|_*} |\bar{A}_c|}{|L^T \bar{A}_c|} \right\|_{\max}.
 \end{aligned}$$

REMARK 3.5. *If the quaternion linear system becomes a real system such that $A_1 X = B_1$, then in (2.10), $\Upsilon_A = \text{diag}(A_1, A_1, A_1, A_1)$, $B_c = [B_1^T, O_n, O_n, O_n]^T$ and the solution $X_c = [X^T, O_n, O_n, O_n]^T$. It also corresponds to (1.1) in which the input matrices have zero imaginary parts that are not perturbed. By Theorems 3.2 and 3.3, we can recover the condition number of real linear system $A_1 X = B_1$ by taking $L^T = I_{4n}$ and letting the parameters α_i, β_i for $i \geq 2$ tend to infinity. The estimate in (3.24) becomes*

$$\kappa^u(A_1, B_1) = \left(\frac{4}{\alpha_1^2} + \frac{1}{\beta_1^2 \|X\|_F^2} \right)^{1/2} \|A_1^{-1}\|_2 \|[\alpha_1 A_1 \ \beta_1 B_1]\|_F.$$

The above upper bound is a little overestimated due to the zero submatrices in X_c . As a matter of fact, the matrix $Q(S_\alpha \otimes I_{n^2})$ in (3.25) takes the form

$$\begin{aligned} \widehat{Q} &:= Q(S_\alpha \otimes I_{n^2}) = ([X^T \ O \ O \ O] \otimes I_{4n})(I_4 \otimes \Pi_{n,4} \otimes I_n)([\alpha_1^{-1}s_1 \ 0 \ 0 \ 0] \otimes I_{n^2}) \\ &= (X^T \otimes I_{4n})[\Pi_{n,4} \otimes I_n \ O \ O \ O][\alpha_1^{-1}\text{vec}(S_1) \otimes I_{n^2} \ O \ O \ O] \\ &= \alpha_1^{-1}(X^T \otimes I_{4n})[(\Pi_{n,4}\text{vec}(S_1e_1) \otimes I_n) \otimes I_n \ O \ O \ O] \\ &= \alpha_1^{-1}((X^T \otimes I_4) \otimes I_n)[(e_1 \otimes I_n) \otimes I_n \ O \ O \ O], \end{aligned}$$

where e_1 is the first column in I_4 . Thus, $\|\widehat{Q}\|_2^2 = \|\widehat{Q}\widehat{Q}^T\|_2 \leq \alpha_1^{-2}\|X\|_2^2$ and the upper bound $\kappa^u(A_1, B_1)$ for the real linear system is modified as

$$\bar{\kappa}^u(A_1, B_1) = \left(\frac{1}{\alpha_1^2} + \frac{1}{\beta_1^2\|X\|_F^2} \right)^{1/2} \|A_1^{-1}\|_2 \|[\alpha_1 A_1 \ \beta_1 B_1]\|_F.$$

This upper bound is exactly the normwise condition number of $A_1X = B_1$. When the right-hand side is single (i.e., $t = 1$), it reduces to the normwise condition number for the single right-hand side system presented in [9].

By taking $L = I_{4n}$, the upper bounds of the mixed and componentwise condition numbers in (3.26)–(3.27) become

$$m^u(A_1, B_1) = \frac{\left\| |A_1^{-1}|(|A_1||X| + |B_1|) \right\|_{\max}}{\|L^T X\|_{\max}}, \quad c^u(A_1, B_1) = \left\| \frac{|A_1^{-1}|(|A_1||X| + |B_1|)}{|L^T X|} \right\|_{\max}.$$

These upper bounds are attainable by simple calculations from (3.19) for $dA_i = 0 (i \geq 2)$. When $t = 1$, they exactly reduce to the mixed and componentwise condition numbers of linear system $A_1x = b$, as also proved in [36]. Similar technique applied to Theorem 3.4 gives the mixed and componentwise condition numbers of A_1^{-1} as

$$m^u(A_1^{-1}) = \frac{\left\| |A_1^{-1}||A_1||A_1^{-1}| \right\|_{\max}}{\|A_1^{-1}\|_{\max}}, \quad c^u(A_1^{-1}) = \left\| \frac{|A_1^{-1}||A_1||A_1^{-1}|}{A_1^{-1}} \right\|_{\max}.$$

They are the same as those in [11, 12, 36].

REMARK 3.6. In Theorem 3.3, if the right-hand side of the quaternion linear system (1.1) is not perturbed, and perturbation only happens on the quaternion matrix A , then the mixed and componentwise condition numbers take the forms as

$$\begin{aligned} m_A(L, A_r, B_r) &= \frac{\| |\mathcal{M}|\text{vec}(|A_r|) \|_\infty}{\|L^T X_c\|_{\max}} \leq \frac{\left\| |L^T \Upsilon_A^{-1}| \Upsilon_{|A|_*} |X_c| \right\|_{\max}}{\|L^T X_c\|_{\max}}, \\ c_A(L, A_r, B_r) &= \left\| \frac{|\mathcal{M}|\text{vec}(|A_r|)}{\text{vec}(L^T X_c)} \right\|_\infty \leq \left\| \frac{|L^T \Upsilon_A^{-1}| \Upsilon_{|A|_*} |X_c|}{|L^T X_c|} \right\|_{\max}. \end{aligned}$$

Likewise, it is obvious that the perturbation only on B leads to the following estimates

$$\begin{aligned} m_B(L, A_r, B_r) &= \frac{\| |\mathcal{N}|\text{vec}(|B_c|) \|_\infty}{\|L^T X_c\|_{\max}} \leq \frac{\left\| |L^T \Upsilon_A^{-1}| |B_c| \right\|_{\max}}{\|L^T X_c\|_{\max}}, \\ c_B(L, A_r, B_r) &= \left\| \frac{|\mathcal{N}|\text{vec}(|B_c|)}{\text{vec}(L^T X_c)} \right\|_\infty \leq \left\| \frac{|L^T \Upsilon_A^{-1}| |B_c|}{|L^T X_c|} \right\|_{\max}. \end{aligned}$$

4. Structured condition numbers for structured matrices. Suppose that $\mathcal{L} \subseteq \mathbb{Q}^{n \times n}$ is a linear subspace which consists of a class of structured quaternion matrices. Specially, if there are $r (r \leq n^2)$ linearly independent real matrices $T_1, \dots, T_r \in \mathcal{L}$, such that for any $A \in \mathcal{L}$, we have

$$(4.28) \quad A = \sum_{i=1}^r g_i T_i,$$

for some $g = [g_1, \dots, g_r]^T \in \mathbb{Q}^r$. Then, an equivalent formulation of (4.28) is

$$(4.29) \quad \text{vec}(A) = \varphi_A^{\text{struct}} g,$$

where the real matrix $\varphi_A^{\text{struct}} = [\text{vec}(T_1) \ \text{vec}(T_2) \ \dots \ \text{vec}(T_r)] \in \mathbb{R}^{n^2 \times r}$. For a general quaternion matrix A without exhibiting any structure, we can take $\varphi_A^{\text{struct}} = I_{n^2}, g = \text{vec}(A)$ in (4.29). Based on the argument from [12, 27, 28], usually the perturbation ΔA has the same structure as A , and hence, there exists a quaternion vector Δg such that $\text{vec}(\Delta A) = \varphi_A^{\text{struct}} \Delta g$.

For simplicity, we assume that each matrix A in \mathcal{L} only depends on a single component of quaternion vector g . Several kinds of structured matrix are included in this category, such as Toeplitz, Hankel, and circulant matrices. For instance, the quaternion circulant matrix associated with a quaternion vector $c = [c_0 \ c_1 \ \dots \ c_{n-1}]^T$ is defined as

$$(4.30) \quad C = \text{circ}(c_0, \dots, c_{n-1}) = \begin{bmatrix} c_0 & c_1 & \dots & c_{n-1} \\ c_{n-1} & c_0 & \dots & c_{n-2} \\ \vdots & \vdots & \dots & \vdots \\ c_1 & c_2 & \dots & c_0 \end{bmatrix}.$$

Obviously, there exist real pattern matrices $Z_0 = I_n, Z_1, \dots, Z_{n-1}$ such that

$$C = c_0 Z_0 + c_1 Z_1 + \dots + c_{n-1} Z_{n-1}.$$

Thus, $\text{vec}(C) = \varphi_C^{\text{struct}} c$ with $\varphi_C^{\text{struct}} = [\text{vec}(Z_0) \ \text{vec}(Z_1) \ \dots \ \text{vec}(Z_{n-1})]$.

In the quaternion linear system (1.1), assume that the right-hand matrix B also has some structure such that

$$\text{vec}(B) = \varphi_B^{\text{struct}} h \quad \text{for} \quad \varphi_B^{\text{struct}} \in \mathbb{R}^{nt \times l},$$

where $h = [h_1 \ \dots \ h_l]^T \in \mathbb{Q}^l$ is some quaternion vector. Then,

$$\text{vec}(A_r) = (I_4 \otimes \varphi_A^{\text{struct}}) g_c, \quad \text{vec}(B_c) = (I_4 \otimes \varphi_B^{\text{struct}}) h_c,$$

where g_c, h_c are column vectors by staking the four parts of quaternion vectors g and h one underneath the other, respectively. Obviously,

$$(4.31) \quad \begin{bmatrix} \text{vec}(A_r) \\ \text{vec}(B_c) \end{bmatrix} = \Psi_{A,B}^{\text{struct}} s, \quad \Psi_{A,B}^{\text{struct}} = \begin{bmatrix} I_4 \otimes \varphi_A^{\text{struct}} & 0 \\ 0 & I_4 \otimes \varphi_B^{\text{struct}} \end{bmatrix},$$

where $s = [g_c^T \ h_c^T]^T$.

Assume that $\text{vec}(\Delta B) = \varphi_B^{\text{struct}} \Delta h$, set $\Delta s = [\Delta g_c^T \ \Delta h_c^T]^T$, then we have

$$(4.32) \quad \begin{bmatrix} \text{vec}(\Delta A_r) \\ \text{vec}(\Delta B_c) \end{bmatrix} = \Psi_{A,B}^{\text{struct}} \Delta s \quad \text{for} \quad \Delta s = \begin{bmatrix} \Delta g_c \\ \Delta h_c \end{bmatrix}.$$

By Theorem 3.1, for structured linear quaternion system (1.1), we have

$$\text{vec}(L^T \Delta X_c) = K^s \Delta s + \mathcal{O}(\|\Delta s\|_2^2) \quad \text{with} \quad K^s = K \Psi_{A,B}^{\text{struct}}.$$

Define the mapping $\phi : \mathbb{R}^{4(t+l)} \rightarrow \mathbb{R}^{kt}$ such that $\phi(s) = \text{vec}(L^T X_c)$; then by the concept of three types of condition numbers in section 1, we have the following theorem.

THEOREM 4.1. *With the notation of Theorem 3.1 and the relations in (4.28)–(4.32), the structured normwise, mixed, and componentwise condition numbers for the quaternion linear system (1.1) take the following form*

$$(4.33) \quad \kappa^s(L, A_r, B_r) = \frac{\|K^s\|_2 \|s\|_2}{\|L^T X_c\|_F},$$

and

$$(4.34) \quad m^s(L, A_r, B_r) = \frac{\| \|K^s\| |s| \|_\infty}{\|L^T X_c\|_{\max}}, \quad c^s(L, A_r, B_r) = \left\| \frac{|K^s| |s|}{\text{vec}(L^T X_c)} \right\|_\infty.$$

THEOREM 4.2. *With the notations of Theorems 3.1–3.3 and the relations in (4.28)–(4.32), let $\mathcal{M}^s = \mathcal{M}(I_4 \otimes \varphi_A^{\text{struct}})$. Then, the structured normwise, mixed, and componentwise condition numbers for the quaternion matrix inverse $\bar{A} := A^{-1}$ take the following form*

$$(4.35) \quad \kappa^s(L, A_r) = \frac{\|\mathcal{M}^s\|_2 \|g_c\|_2}{\|L^T \bar{A}_c\|_F},$$

and

$$(4.36) \quad m^s(L, A_r) = \frac{\| \|\mathcal{M}^s\| |g_c| \|_\infty}{\|L^T \bar{A}_c\|_{\max}}, \quad c^s(L, A_r) = \left\| \frac{|\mathcal{M}^s| |g_c|}{\text{vec}(L^T \bar{A}_c)} \right\|_\infty.$$

REMARK 4.3. *For the quaternion linear system (1.1), if perturbations only happen on the matrix A , then the structured mixed and componentwise condition numbers reduce to*

$$\kappa_A^s = \frac{\|\mathcal{M}^s\|_2 \|g_c\|_2}{\|L^T X_c\|_F}, \quad m_A^s = \frac{\| \|\mathcal{M}^s\| |g_c| \|_\infty}{\|L^T X_c\|_{\max}}, \quad c_A^s = \left\| \frac{|\mathcal{M}^s| |g_c|}{\text{vec}(L^T X_c)} \right\|_\infty.$$

The perturbation only on B gives the structured condition numbers as

$$\kappa_B^s = \frac{\|\mathcal{N}^s\|_2 \|h_c\|_2}{\|L^T X_c\|_F}, \quad m_B^s = \frac{\| \|\mathcal{N}^s\| |h_c| \|_\infty}{\|L^T X_c\|_{\max}}, \quad c_B^s = \left\| \frac{|\mathcal{N}^s| |h_c|}{\text{vec}(L^T X_c)} \right\|_\infty,$$

where $\mathcal{N}^s = \mathcal{N}(I_4 \otimes \varphi_B^{\text{struct}})$.

REMARK 4.4. *Note that in (4.33)–(4.36), $K^s = [\mathcal{M}^s \quad \mathcal{N}^s]$ and*

$$\begin{aligned} \mathcal{M}^s &= -(I_t \otimes (L^T \Upsilon_A^{-1}) Q([\text{vec}(S_1) \quad \dots \quad \text{vec}(S_4)] \otimes [\text{vec}(T_1) \quad \text{vec}(T_2) \quad \dots \quad \text{vec}(T_r)])) \\ &= -(L^T \Upsilon_A^{-1}) [\eta_1^{(1)} \quad \dots \quad \eta_r^{(1)} \quad \eta_1^{(2)} \quad \dots \quad \eta_r^{(2)} \quad \dots \quad \eta_1^{(4)} \quad \dots \quad \eta_r^{(4)}], \end{aligned}$$

where $\eta_i^{(j)} = \text{vec}((S_j \otimes T_i) X_c)$ with $(S_j \otimes T_i)$ being a block component of Υ_{T_i} . In the expression of $\eta_i^{(j)}$, $(S_j \otimes T_i) X_c$ can be computed in Kronecker product-free manner, which needs much cheaper cost than direct formulation of \mathcal{M}^s . The same goes for the computation of \mathcal{N}^s if $\varphi_B^{\text{struct}}$ has some linear structure.

5. Numerical experiments. In this section, we will test the condition numbers in estimating the forward error bounds of quaternion linear system (1.1) and quaternion matrix inverse. All the computations are carried out using Matlab R2012b with the machine precision $\epsilon_M = 2.2 \times 10^{-16}$.

EXAMPLE 5.1. The aim of this example is to verify the effectiveness of the condition numbers of quaternion linear system and quaternion matrix inverse. Let the quaternion matrix A be constructed as

$$(5.37) \quad A = YDZ^* \in \mathbb{Q}^{n \times n}, \quad Y = I_n - 2yy^*, \quad Z = I_n - 2zz^*,$$

where $y, z \in \mathbb{Q}^n$ are random unit quaternion vectors, and $D = \text{diag}(1, 1/2, \dots, 1/(n-1), \delta) \in \mathbb{R}^{n \times n}$ with $0 < \delta \leq \frac{1}{n}$. Here, $\kappa = \delta^{-1}$ is used to control the condition number of A . Take B_c to be a random $4n \times t$ matrix whose entries are uniformly distributed on the interval $[0, 1]$.

Set

$$(5.38) \quad \Delta A_c = 10^{-10} \cdot A_c \odot \text{rand}(4n, n), \quad \Delta B_c = 10^{-10} \cdot B_c \odot \text{rand}(4n, 1),$$

where \odot denotes the entrywise multiplication of two matrices with the same size. Let $\Delta X_c = \tilde{X}_c - X_c$ be the error of the solutions between the perturbed and original problem. Here, the solutions are obtained via the partial pivoting real structure-preserving LU algorithm [24].

Choose $L = L_0 = I_{4n}$. Set

$$(5.39) \quad \gamma_\kappa = \frac{\|L^T \Delta X_c\|_F}{\|L^T X_c\|_F}, \quad \gamma_m = \frac{\|L^T \Delta X_c\|_\infty}{\|L^T X_c\|_\infty}, \quad \gamma_c = \left\| \frac{L^T \Delta X_c}{L^T X_c} \right\|_\infty,$$

and

$$(5.40) \quad \epsilon_1 := \frac{\|[\Delta A_r \ \Delta B_r]\|_F}{\|[A_r \ B_r]\|_F}, \quad \epsilon_2 := \min\{\epsilon : \|[\Delta A_r \ \Delta B_r]\| \leq \epsilon \|[A_r \ B_r]\|\}.$$

We can get the upper bounds of $\gamma_\kappa, \gamma_m, \gamma_c$ as $\epsilon_1 \kappa(\epsilon_1 \kappa^u), \epsilon_2 m(\epsilon_2 m^u), \epsilon_2 c(\epsilon_2 c^u)$, respectively, where κ, m, c denote the normwise, mixed, and componentwise condition numbers, respectively, and κ^u, m^u, c^u are, respectively, the upper bounds of κ, m, c given in Theorems 3.2 and 3.3.

In Table 1, we compare the approximate upper bounds with the corresponding relative errors of the solution to (1.1). It can be seen that for the normwise condition number, the upper bound κ^u approximates κ well in all cases, up to a factor about 10; m^u and c^u approximate better to m and c , respectively. However, when n increases from 30 to 90 and κ increases from 10^2 to 10^6 , the approximate upper bounds based on mixed and componentwise condition numbers are as sharp as the actual forward errors, while the normwise condition number-based upper bounds tend to be much farther away from the actual forward errors. That is partly because the problem becomes ill-conditioned by the estimate in Theorem 3.2, where according to (2.9), $\|\Upsilon_A^{-1}\|_2 = \|\Upsilon_{A^{-1}}\|_2 = \|A^{-1}\|_2$ becomes large when κ increases. Another reason might be that when n is large, the algorithm produces a large backward rounding error (measured in norm) in the partial pivoting quaternion LU (see [24]). Combined the backward error with the condition number, the case with $n = 90$ and $\kappa = 10^6$ gives the worst estimate of the forward error of the solution.

For the forward error of quaternion matrix inverse, by setting $X_c = \bar{A}_c$ and restricting the perturbations only on A (i.e., setting B_r and its perturbation ΔB_r to be zero matrices in (5.39)–(5.40), and for the ease of distinguishment, we use the superscript A on a series of notation associated with γ and ϵ), we get the actual relative forward errors and their bounds in Table 2, where the random 15×15 matrix A is generated

as (5.37)–(5.38). The results show that the estimated bounds based on three condition numbers are usually one or two orders higher than the actual relative errors. This means that for equilibratory input data, the condition numbers-based bounds are reliable in estimating the relative forward error of quaternion matrix inverse.

TABLE 1
 Comparison of approximate upper bounds with the corresponding relative forward errors for quaternion linear system

n	$n = 30, t = 3$			$n = 60, t = 3$			$n = 90, t = 3$		
	10^2	10^4	10^6	10^2	10^4	10^6	10^2	10^4	10^6
γ_κ	6.9e-11	5.0e-09	3.4e-07	5.3e-11	1.0e-09	1.6e-07	5.3e-11	2.1e-10	6.9e-08
$\epsilon_1 \kappa$	6.1e-08	6.7e-06	6.5e-04	8.4e-08	9.3e-06	9.1e-04	9.8e-08	1.1e-05	1.1e-03
$\epsilon_1 \kappa^u$	1.2e-07	1.2e-05	1.2e-03	1.7e-07	1.7e-05	1.8e-03	2.0e-07	2.0e-05	2.2e-03
γ_m	7.9e-11	6.3e-09	3.1e-07	4.2e-11	9.6e-10	1.5e-07	5.9e-11	2.0e-10	6.3e-08
$\epsilon_2 m$	2.9e-09	1.3e-07	1.9e-05	1.7e-09	4.8e-08	3.4e-06	1.8e-09	2.3e-08	2.5e-06
$\epsilon_2 m^u$	4.9e-09	2.1e-07	3.4e-05	2.9e-09	7.6e-08	5.8e-06	3.0e-09	3.6e-08	4.1e-06
γ_c	7.9e-11	6.3e-09	3.1e-07	4.2e-11	9.6e-10	1.5e-07	5.9e-11	2.0e-10	6.3e-08
$\epsilon_2 c$	2.9e-09	1.3e-07	1.9e-05	1.7e-09	4.8e-08	3.4e-06	1.8e-09	2.3e-08	2.5e-06
$\epsilon_2 c^u$	4.9e-09	2.1e-07	3.4e-05	2.9e-09	7.6e-08	5.8e-06	3.0e-09	3.6e-08	4.1e-06

TABLE 2
 Comparison of approximate upper bounds with the corresponding relative forward errors for quaternion matrix inverse

δ	γ_κ^A	$\epsilon_1^A \kappa^A$	$\epsilon_1^A \kappa^{A^u}$	γ_m^A	$\epsilon_1^A m^A$	$\epsilon_1^A m^{A^u}$	γ_c^A	$\epsilon_1^A c^A$	$\epsilon_1^A c^{A^u}$
10^{-2}	1.54e-10	8.96e-09	1.63e-08	1.03e-10	2.34e-09	2.75e-09	2.28e-07	1.25e-05	1.89e-05
10^{-4}	1.15e-08	8.96e-07	1.71e-06	1.01e-08	2.57e-07	3.03e-07	1.18e-04	7.02e-03	9.75e-03
10^{-6}	1.14e-06	8.96e-05	1.71e-04	1.01e-06	2.57e-05	3.03e-05	1.18e+00	7.03e+01	9.76e+01

EXAMPLE 5.2. In this example, we test the condition numbers of the linear problem with badly scaled coefficient matrix. For the choice of L , we set $L_0 = I_{4n}$ and use the matrices L_{\max} , L_{\min} to pick the rows with maximal and minimal infinite norms in X_c , respectively. Let $n = 4, t = 1, X_1 = [10^{-4}, 10^{-4}, 1, 1]^T$, $X_i = X_1, A_i = A_1$ for $i \geq 2$, where

$$A_1 = \begin{bmatrix} \delta & 0 & 0 & 0 \\ 0 & \delta & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}, \quad B_c = \Upsilon_A X_c = \Upsilon_A \begin{bmatrix} X_1 \\ X_2 \\ X_3 \\ X_4 \end{bmatrix},$$

and $\delta > 0$ is a tiny parameter.

With the componentwise perturbation as in (5.38) and the notation in (5.39)–(5.40), in Table 3, it can be seen that for each given δ , the upper bound κ^u approximates κ very well. However, for the estimate based on normwise condition number, there is a big difference between the estimated value and the real value for varying matrix L . The upper bounds of the row with maximal infinite norm in the solution are sharp, while the estimate of the rows with minimal infinite norm in the solution is not satisfactory, even the parameter δ is not very small.

When δ decreases to 10^{-4} or 10^{-6} and the linear system becomes sparse and badly scaled, the normwise condition number-based upper bounds tend to be much farther away from the actual forward errors. On

the other hand, the approximate upper bounds via mixed and componentwise condition numbers are as sharp as the actual forward errors. The sharp estimate is because the high-magnitude entries in Υ_A^{-1} (say, for $\delta = 10^{-6}$, the maximal absolute value in Υ_A^{-1} is $2.5e+6$) is restrained by small or zeros values in $|A_r|$ and $|B_c|$ through the entrywise multiplication. However, the normwise condition number is controlled by the high-magnitude entries in Υ_A^{-1} , even there are small entries in $|A_r|$ and $|B_c|$, they do not play much role in inhibiting the magnitude of $\|\Upsilon_A^{-1}\|_2$. It is precisely because of this that the normwise condition number in Example 5.1 gives worse estimates of the forward errors of the solution when $n = 90, t = 3$ and $\kappa = 10^6$.

TABLE 3
 Comparison of approximate upper bounds with the corresponding relative forward errors

δ	10^{-2}			10^{-4}			10^{-6}		
	L_0	L_{\max}	L_{\min}	L_0	L_{\max}	L_{\min}	L_0	L_{\max}	L_{\min}
γ_κ	3.1e-11	1.9e-11	2.6e-11	3.8e-11	2.0e-11	2.6e-11	5.8e-11	3.6e-11	4.3e-11
$\epsilon_1\kappa$	1.8e-08	4.5e-10	4.6e-04	2.3e-06	6.3e-10	6.8e-02	2.3e-04	4.5e-10	4.6e+00
$\epsilon_1\kappa^u$	3.4e-08	8.6e-10	8.9e-04	4.4e-06	1.2e-09	1.3e-01	4.3e-04	8.5e-10	8.8e+00
γ_m	4.6e-11	1.9e-11	2.6e-11	7.4e-11	2.0e-11	2.6e-11	1.0e-10	3.6e-11	4.3e-11
ϵ_2m	2.8e-10	2.8e-10	2.8e-10	3.0e-10	2.8e-10	3.0e-10	3.0e-10	2.8e-10	2.9e-10
ϵ_2m^u	5.5e-10	5.5e-10	5.6e-10	5.9e-10	5.6e-10	6.0e-10	6.0e-10	5.7e-10	5.8e-10
γ_c	4.6e-11	1.9e-11	2.6e-11	7.4e-11	2.0e-11	2.6e-11	1.0e-10	3.6e-11	4.3e-11
ϵ_2c	2.8e-10	2.8e-10	2.8e-10	3.0e-10	2.8e-10	3.0e-10	3.0e-10	2.8e-10	2.9e-10
ϵ_2c^u	5.5e-10	5.5e-10	5.6e-10	5.9e-10	5.6e-10	6.0e-10	6.0e-10	5.7e-10	5.8e-10

EXAMPLE 5.3. Consider the quaternion linear system (1.1) in which the coefficient matrix is a quaternion circulant matrix taking the form (4.30). Set the quaternion matrix $C = C_1 + C_1i + C_1j + C_1k$ and take $A = C^{-1}$, where $C_1 = \text{circ}(c)$ is a real circulant matrix [28] generated from the $n \times 1$ vector

$$c = [1 \quad 1 \quad \dots \quad 1 \quad c_n]^T, \text{ with } c_n = -(n - 1) + \delta(0 < \delta < 1).$$

It is easy to show that

$$A = \frac{1}{4}(C_1^{-1} - C_1^{-1}i - C_1^{-1}j - C_1^{-1}k) = \frac{1}{4}C_1^{-1}(1 - i - j - k),$$

where $C_1^{-1} = \text{circ}(\bar{c})$ with $\bar{c}_i = -1/\xi$ for $i \neq 2$ and $\xi = (c_n - 1)(c_n + n - 1)$, and $\bar{c}_2 = (c_n + n - 2)/\xi$. Hence, $\bar{c}_i = \mathcal{O}(n^{-1}\delta^{-1})$ and the magnitude of \bar{c} increases with the decrease of δ . Take $n = 10, t = 1$ and $L_0 = I_{4n}$. For given X_c , generate a $4n \times 1$ vector $B_c = \Upsilon_A X_c$. Restrict the perturbations only on A where the vector c is perturbed to $\tilde{c} = c \odot (1 + 10^{-5} * \text{rand}(1, n))$.

In (4.29), it is obvious that $g = \frac{1}{4}(1 - i - j - k)\bar{c}$ and $|g_c| = \frac{1}{4}e \otimes \bar{c}$ with $e = [1, 1, 1, 1]^T$ and $\bar{c} > 0$. Define

$$\epsilon_1^s = \frac{\|\Delta g_c\|_2}{\|g_c\|_2}, \quad \epsilon_2^s = \min\{\epsilon : |\Delta g_c| \leq \epsilon |g_c|\}.$$

In Table 4, we compare the upper bounds based on unstructured and structured condition numbers with the actual relative forward errors. It is observed that when X_c is a fixed random vector, the advantage of structured condition numbers over the unstructured ones is weak, while for the all-one vector $X_c = e$, especially when δ is close to zero, the structured condition numbers behave much better than the unstructured ones. In this case, even the unstructured mixed/componentwise condition numbers fail to estimate the

forward errors well. The experimental results illustrate that the corresponding problem with $X_c = e$ is well-conditioned. The well-condition can also be observed from structured condition number formulae in Remarks 4.3–4.4 in that

$$|\mathcal{M}^s|_{|g_c|} \leq \frac{1}{4} |\Upsilon_A^{-1}| \sum_{j=1}^4 (|S_j| \otimes \sum_{i=1}^n (\bar{c}_i T_i)) e = |\Upsilon_{A^{-1}}| |\Upsilon_{|A|_*}| e,$$

where $\sum_{i=1}^n (\bar{c}_i T_i) = \bar{C} = C_1^{-1}$ is a nonnegative matrix, $|A|_* = \frac{1}{4} C_1^{-1} (1 + i + j + k)$ with $C_1 e = \delta e$ and $C_1^{-1} e = \delta^{-1} e$. It follows that

$$|\Upsilon_{|A|_*}| e = \delta^{-1} e, \quad |\Upsilon_{A^{-1}}| e = 4\delta e,$$

from which we derive that the mixed condition number $m_A^s \leq 4$, and hence, the corresponding system is well-conditioned.

TABLE 4

Comparison of upper bounds based on structured and unstructured condition numbers with the corresponding relative forward errors

X_c	$X_c = \text{rand}(4n, 1)$			$X_c = [1, 1, \dots, 1]^T$		
	10^0	10^{-2}	10^{-4}	10^0	10^{-2}	10^{-4}
γ_k	5.70e-06	3.91e-04	3.98e-02	4.82e-06	4.38e-06	4.38e-06
$\epsilon_1 \kappa_A$	4.61e-05	5.02e-03	5.03e-01	5.44e-05	5.44e-03	5.44e+01
$\epsilon_1^s \kappa_A^s$	5.05e-05	5.50e-03	5.50e-01	2.42e-05	2.18e-05	2.18e-05
γ_m	7.53e-06	5.65e-04	5.58e-02	4.82e-06	4.38e-06	4.38e-06
$\epsilon_2 m_A$	1.63e-04	1.70e-02	1.70e+00	3.18e-04	3.36e-02	3.36e+02
$\epsilon_2^s m_A^s$	1.61e-04	1.72e-02	1.72e+00	7.48e-05	7.48e-05	7.48e-05
γ_c	1.50e-04	2.83e-02	2.65e+00	4.82e-06	4.38e-06	4.38e-06
$\epsilon_2 c_A$	2.07e-02	2.19e+00	2.19e+02	3.18e-04	3.36e-02	3.36e+02
$\epsilon_2^s c_A^s$	1.61e-04	1.72e-02	1.72e+00	7.48e-05	7.48e-05	7.48e-05

6. Conclusion and further work. In this paper, we investigate the structured and unstructured condition numbers of quaternion matrix inverse and quaternion linear system with multiple right-hand sides. By making use of the Kronecker product operations and real counterpart of quaternion matrices, the first-order perturbation of the solution of the quaternion linear system is analyzed, from which the closed formula for the normwise, mixed, and componentwise condition numbers of the quaternion linear system are derived. In order to avoid the large storage and computational cost for computing these condition numbers, upper bounds with compact forms are given. These closed formulae and compact upper bounds include the existing results for the real linear system and real matrix inverse. Numerical results show that the compact upper bounds are tight, compared with the actual condition numbers. It is also shown that for badly scaled matrix, mixed and componentwise condition numbers are preferred to estimate the forward errors. We also analyze the structured condition numbers for the structured linear system. In estimating the forward error of the solution to some specific structured problem, structured condition numbers are shown to be much tighter than the unstructured ones.

When the coefficient and right-hand side matrices in the quaternion linear system are rectangular, it is of interest to discuss the condition numbers of quaternion least squares problem. We will study this issue in a separate paper [25] to unify those results for real least squares problems.

Acknowledgements. The authors are grateful to the handling editor and two anonymous referees for their useful comments and suggestions, which greatly improved the original presentation.

Conflict of interest. The authors declare that they have no conflict of interest in the manuscript.

REFERENCES

- [1] T.T. Chen and W. Li. On condition numbers for the weighted Moore-Penrose inverse and the weighted least squares problem involving Kronecker products. *E. Asian J. Appl. Math.*, 4(1):1–20, 2014.
- [2] F. Cucker, H.A. Diao, and Y.M. Wei. On mixed and componentwise condition numbers for Moore-Penrose inverse and linear least squares problems. *Math. Comput.*, 76:947–963, 2007.
- [3] S. De Leo and P. Rotelli. Quaternion scalar field. *Phys. Rev. D*, 45:575–579, 1992.
- [4] H.A. Diao, W.G. Wang, and Y.M. Wei. On condition numbers for Moore-Penrose inverse and linear least squares problem involving Kronecker products. *Numer. Linear Algebra Appl.*, 20(1):44–59, 2013.
- [5] D. Finkelstein, J.M. Jauch, S. Schiminovich, and D. Speiser. Foundations of quaternion quantum mechanics. *J. Math. Phys.* 3:207–220, 1962.
- [6] A.J. Geurts. A contribution to the theory of condition. *Numer. Math.*, 39:85–96, 1982.
- [7] I. Gohberg and I. Koltracht. Mixed, componentwise, and structured condition numbers. *SIAM J. Matrix Anal. Appl.*, 14:688–704, 1993.
- [8] A. Graham. *Kronecker Products and Matrix Calculus with Application*. Wiley, New York, 1981.
- [9] S. Gratton. On the condition number of linear least squares problems in weighted Frobenius norm. *BIT*, 36(3):523–530, 1996.
- [10] W.R. Hamilton. *Elements of Quaternions*. Chelsea, New York, 1969.
- [11] N.J. Higham. A survey of componentwise perturbation theory in numerical linear algebra. *Proc. Symposia Appl. Math.*, 48:49–77, 1994.
- [12] N.J. Higham. *Accuracy and Stability of Numerical Algorithms*, 2nd edn. SIAM, Philadelphia, PA, 2002.
- [13] Z.G. Jia. *The Eigenvalue Problem of Quaternion Matrix: Structure-preserving Algorithms and Applications*. Science Press, Beijing, 2019.
- [14] Z.G. Jia, K. Ng Michael and G.J. Song. Lanczos method for large-scale quaternion singular value decomposition. *Numer. Algor.*, 82(2):699–717, 2019.
- [15] Z.G. Jia, K. Ng Michael, and G.J. Song. Robust quaternion matrix completion with applications to image inpainting. *Numer. Linear Algebra Appl.*, 26(4):e2245, 2019.
- [16] Z.G. Jia, K. Ng Michael, and W. Wang. Color image restoration by saturation-value total variation. *SIAM J. Imaging Sci.*, 12(2):972–1000, 2019.
- [17] Z.G. Jia, M.S. Wei, and S.T. Ling. A new structure-preserving method for quaternion Hermitian eigenvalue problems. *J. Comput. Appl. Math.*, 239:12–24, 2013.
- [18] Z.G. Jia, M.S. Wei, M.X. Zhao, and Y. Chen. A new real structure-preserving quaternion QR algorithm. *J. Comput. Appl. Math.*, 343:26–48, 2018.
- [19] W.H. Kang and H. Xiang. Level-2 condition numbers for least-squares solution of Kronecker product linear systems. *Int. J. Comput. Math.*, 85(5):827–841, 2008.
- [20] A.N. Langville and W.J. Stewart. The Kronecker product and stochastic automata networks. *J. Comput. Appl. Math.*, 167:429–447, 2004.
- [21] Y. Li, M.S. Wei, F.X. Zhang, and J.L. Zhao. A real structure-preserving method for the quaternion LU decomposition, revisited. *Calcolo*, 54(4):1553–1563, 2017.
- [22] Y. Li, M.S. Wei, F.X. Zhang, and J.L. Zhao. A fast structure-preserving method for computing the singular value decomposition of quaternion matrix. *Appl. Math. Comput.*, 235:157–167, 2014.
- [23] Y. Li, M.S. Wei, F.X. Zhang, and J.L. Zhao. Real structure-preserving algorithms of Householder based transformations for quaternion matrices. *J. Comput. Appl. Math.*, 305:82–91, 2016.

- [24] Q.H. Liu, Q. Zhang and X.J. Xu. Accuracy and stability of quaternion Gaussian elimination. *Numer. Algor.*, 2023. <https://doi.org/10.1007/s11075-023-01531-y>.
- [25] Q.H. Liu and S. Wang. On condition numbers of quaternion least squares problems. Technical Report, Shanghai University, 2023.
- [26] J.R. Rice. A theory of condition. *SIAM J. Numer. Anal.*, 3:287–310, 1966.
- [27] S.M. Rump. Structured perturbations part I: normwise distances. *SIAM J. Matrix Anal. Appl.*, 25:1–30, 2003.
- [28] S.M. Rump. Structured perturbations part II: componentwise distances. *SIAM J. Matrix Anal. Appl.*, 25:31–56, 2003.
- [29] S. Sangwine and N. Le Bihan. *Quaternion Toolbox for Matlab*. <http://qtfm.sourceforge.io/>.
- [30] G. Sclarici and L. Solombrino. Notes on quaternionic groups representation. *Int. J. Theor. Phys.*, 34:2491–2500, 1995.
- [31] G. Sclarici and L. Solombrino. Quaternionic representation of magnetic groups. *J. Math. Phys.*, 38:1147–1160, 1997.
- [32] M.H. Wang and W.H. Ma. A structure-preserving method for the quaternion LU decomposition in quaternionic quantum theory. *Comput. Phy. Commun.*, 184:2182–2186, 2013.
- [33] Y.M. Wei, H.A. Diao, and S.Z. Qiao. Condition number for weighted linear least squares problem. *J. Comput. Math.*, 25(5):561–572, 2007.
- [34] M.S. Wei, Y. Li, F.X. Zhang, and J.L. Zhao. *Quaternion Matrix Computations*. Nova Science Publishers, New York, 2018.
- [35] H. Xiang, H.A. Diao, and Y.M. Wei. On perturbation bounds of Kronecker product linear systems and their level-2 condition numbers. *J. Comput. Appl. Math.*, 183:210–231, 2005.
- [36] H. Xiang and Y.M. Wei. Structured mixed and componentwise condition numbers of some structured matrices. *J. Comput. Appl. Math.*, 202:217–229, 2007.
- [37] H. Yang and S.X. Wang. A flexible condition number for weighted linear least squares problem and its statistical estimation. *J. Comput. Appl. Math.*, 292:320–328, 2016.
- [38] F.Z. Zhang. Quaternions and matrices of quaternion. *Linear Algebra Appl.*, 251:21–57, 1997.
- [39] H.M. Zhang, H. Xiang, and Y.M. Wei. Condition numbers for linear systems and Kronecker product linear systems with multiple right-hand sides. *Int. J. Comput. Math.*, 84(12):1805–1817, 2007.