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A NUMERICALLY STABLE BLOCK MODIFIED GRAM-SCHMIDT ALGORITHM FOR SOLVING STIFF WEIGHTED LEAST SQUARES PROBLEMS *

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Abstract

Recently, Wei in [18] proved that perturbed stiff weighted pseudoinverses and stiff weighted least squares problems are stable, if and only if the original and perturbed coefficient matrices A and $\overline{A}$ satisfy several row rank preservation conditions. According to these conditions, in this paper we show that in general, ordinary modified Gram-Schmidt with column pivoting is not numerically stable for solving the stiff weighted least squares problem. We then propose a row block modified Gram-Schmidt algorithm with column pivoting, and show that with appropriately chosen tolerance, this algorithm can correctly determine the numerical ranks of these row partitioned sub-matrices, and the computed QR factor $\overline{R}$ contains small roundoff error which is row stable. Several numerical experiments are also provided to compare the results of the ordinary Modified Gram-Schmidt algorithm with column pivoting and the row block Modified Gram-Schmidt algorithm with column pivoting.

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1. Introduction

In this paper, we use the following notations. $\Re^{m\times n}$ is the set of all $m\times n$ matrices with real entries, $\Re_r^{m\times n}$ is a subset of $\Re^{m\times n}$ in which any matrix has rank r. For a given matrix A, A^T is the transpose of A. I and 0 respectively denote the identity and zero matrices with appropriate sizes, e_k is the kth column of the identity matrix I,$e=[1,\cdots,1]$ is a vector with appropriate size, $\|\cdot\|\equiv\|\cdot\|_2$ is the Euclidean vector norm or corresponding subordinate matrix norm. The line over a quantity is the corresponding a perturbed version.

We are concerned with the numerical computations of the stiff weighted least squares (stiff WLS) problem

$$\min_{x\in\Re^n}\|W^{\frac{1}{2}}(Ax-b)\|=\min_{x}\|D(Ax-b)\|, \tag{1}$$

where $A\in R^{m\times n}, b\in R^m$ are a known coefficient matrix and observation vector, respectively, and

$$D=\operatorname{diag}(d_{11},d_{22},\cdots,d_{mm})=\operatorname{diag}(w_{11}^{\frac{1}{2}},w_{22}^{\frac{1}{2}},\cdots,w_{mm}^{\frac{1}{2}})=W^{\frac{1}{2}} \tag{2}$$

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is the weight matrix in which the scalar parameters $d_1, \cdots, d_m$ vary widely in size. The stiff WLS problem (1) is widely used, e.g., in electronic networks, certain classes of finite element problems, the interior point method for constrained optimization (e.g., see [12]), and for solving the equality constrained least squares problem (e.g., see [1, 13, 14]),

$$\min_{x\in\Re^n} \|Kx - g\| \quad \text{s.t.} \quad Lx = h,$$

by the method of weighting,

$$\min_x \left\| \begin{pmatrix} \tau L \\ K \end{pmatrix} x - \begin{pmatrix} \tau h \\ g \end{pmatrix} \right\|,$$

where τ is a large parameter; one usually chooses $\tau \sim u^{-\frac{1}{2}}$ with u the machine roundoff unit.

The upper bound and the stability of weighted pseudoinverses and WLS problems are very important subjects in areas like numerical linear algebra and optimization, especially after the appearance of the famous paper of Karmarkar [8] which introduced the interior point method for solving optimization problems. The authors of [11, 10, 15, 16, 6] studied the supremum of the weighted pseudoinverses.

Wei [15, 16], Wei and De Pierro [19] proved that when W ranges over $\mathcal{D}$ that is a set of positive definite diagonal matrices, the perturbations are stable to weighted pseudoinverses $A_W^\dagger \equiv (W^{\frac{1}{2}}A)^\dagger W^{\frac{1}{2}}$ and corresponding WLS problems, *if and only if any* $\mathrm{rank}(A)$ *rows of the matrix* A *are linearly independent.*

In practical scientific computations, the above condition is too restrictive to hold, and the weight matrix W is usually fixed and severely stiff. In [17], Wei found that the stiff weighted pseudoinverse is close to a related multi-level constrained pseudoinverse $A_C^\dagger$ and the solution set of Eq. (1) is close to a related multi-level constrained least squares problem. Based on this observation, Wei [18] derived the stability conditions of perturbed stiff weighted pseudoinverses and stiff WLS problems.

Without loss of generality, we make the following notation and assumptions for the matrices A and W.

Assumption 1.1. The matrices A and W in Eq. (1) satisfy the following conditions: $\|A(i,:)\|$ have the same order for $i = 1, \cdots, m$, $w_1 > w_2 > \cdots > w_k > 0$, $m_1 + m_2 + \cdots + m_k = m$, and we denote $W = \mathrm{diag}(w_1 I_{m_1}, w_2 I_{m_2}, \cdots, w_k I_{m_k})$,

$$A = \begin{pmatrix} A_1 \\ \vdots \\ A_k \end{pmatrix} \begin{matrix} m_1 \\ \vdots \\ m_k \end{matrix}, \quad C_j = \begin{pmatrix} A_1 \\ \vdots \\ A_j \end{pmatrix}, \quad j = 1, \cdots, k,$$

and assume

$$0 < \epsilon_{ij} \equiv w_i/w_j \ll 1, \text{ for } 1 \le j < i \le k \text{ so } \epsilon = \max_{1\le j<k} \{\epsilon_{j+1,j}\} \ll 1.$$

We also set

$$P_0 = I_n, \quad P_j = I - C_j^\dagger C_j, \quad \mathrm{rank}(C_j) = r_j, \quad j = 1, \cdots, k.$$

With above mentioned matrices A, A_j, C_j and the parameters ϵ_{ij}, denote $\overline{A}$, $\overline{A}_j$, $\overline{C}_j$, $\overline{\epsilon}_{ij}$ as the perturbed versions of A, A_j, C_j, ϵ_{ij}, respectively. Then Wei (in Theorems 3.1–3.5, 4.1-4.2 of [18]) proved the following results.

Theorem 1.1. *Suppose that A and W are given matrices satisfying the notation and conditions in Assumption 1.1. Then perturbed stiff pseudoinverses and perturbed stiff WLS problems are stable, if and only if*

$$\text{rank}(\overline{C}_j) = \text{rank}(C_j) = r_j, \quad j = 1, 2, \cdots, k. \tag{3}$$

- *1. If the conditions of Eq. (3) hold, and $E \cdot \|A_W^\dagger\| < 1$ with*

$$E \equiv \|\delta A\| + \|A\| \cdot \|B_\epsilon^\dagger\| \cdot \Big[\frac{\nu\epsilon}{1-\epsilon} \max_{1\le j<i\le k} \|A_i Q_j\| + \frac{1}{1-\epsilon(1+\nu)} \max_{1\le j\le i\le k} (\|\delta A_i\| + 2\sqrt{2}\|A_i\| \cdot \|C_j^\dagger \delta C_j\|)\Big],$$

  where

$$\nu = \max_{1\le j<i\le k} |\overline{\epsilon}_{ij} - \epsilon_{ij}|/\epsilon_{ij},$$

  then we have the following estimates:

$$\|\overline{A}_{\overline{W}}^\dagger\| \le \frac{\|A_W^\dagger\|}{1 - E \cdot \|A_W^\dagger\|},$$
$$\|\overline{A}_{\overline{W}}^\dagger - A_W^\dagger\| \le \frac{\sqrt{5}+1}{2} \cdot E \cdot \frac{\|A_W^\dagger\|^2}{1 - E \cdot \|A_W^\dagger\|}.$$

- *2. If $\text{rank}(A) < \min\{m,\ n\}$ and we allow*

$$\text{rank}(\overline{A}) > \text{rank}(A),$$

  then for any value $0 < \xi \ll 1$, there exists a perturbed matrix

$$\overline{A} = A + \delta A$$

  satisfying $\|\delta A\| = \xi$, $\text{rank}(\overline{A}) > \text{rank}(A)$, such that

$$\|\overline{A}_W^\dagger\| \ge \frac{1}{\xi} \quad \textit{and} \quad \|\overline{A}_W^\dagger - A_W^\dagger\| \ge \frac{1}{\xi}.$$

- *3. Let $M_i = \sum_{j=1}^i m_j$. We enforce the condition $\text{rank}(A) = \text{rank}(\overline{A}) \le \min\{m, n\}$, and suppose that there exists an integer i with $1 \le i < k$, such that*

$$\text{rank}(C_{i-1}) = M_{i-1},\ \textit{rank}(C_i) < \min\{M_i, n\} \le n.$$

  Let l be the largest integer satisfying $k \ge l > i$ and

$$\text{rank}(C_{l-1}) < n, \text{rank}(C_l) = n.$$

  If we allow

$$\text{rank}(\overline{C}_i) > \text{rank}(C_i),$$

  then for any value $0 < \xi \ll 1$, there exists a perturbed matrix $\overline{A} = A + \delta A$ satisfying $\|\delta A\| = \xi$, $\text{rank}(\overline{A}) = \text{rank}(A) = n$, such that

$$\|\overline{A}_W^\dagger\|_2 \ge \frac{\xi}{\xi^2 + a\epsilon_{li}}, \qquad \|\overline{A}_W^\dagger - A_W^\dagger\|_2 \ge \frac{\xi}{\xi^2 + a\epsilon_{li}},$$

  where $a > 0$ is a constant independent of ξ.

Based on the above stable conditions for perturbed stiff weighted pseudoinverses and stiff WLS problems, we propose a numerically stable row block modified Gram-Schmidt (MGS) algorithm with column pivoting. We show that with appropriately chosen tolerance, this algorithm can correctly determine the numerical ranks of these row partitioned sub-matrices, and computed QR factor $\overline{R}$ contains small roundoff error therefore is also row-wise stable.

Notice that for the MGS, one needs to perform column pivoting to ensure that the algorithm can correctly determine the numerical rank of the matrix A and has backward roundoff stability [2, 3, 4]. On the other hand, from the stability conditions mentioned in Eq. (3), it is not enough only to perform column pivoting for numerical stability when solving stiff WLS problem Eq. (1). To see this, let us consider the following example.

Example 1.1. Suppose that

$$A = \begin{pmatrix} -4 & 2 & -3 \\ 4 & 2 & 2 \\ 2 & 1 & 1 \\ 1 & -1 & 1 \end{pmatrix}, \ b = \begin{pmatrix} -9 \\ 4 \\ 1 \\ 4 \end{pmatrix}, \ D = \mathrm{diag}(1, 1, 10^{-2}, d).$$

Then $\mathrm{rank}(A) = 3$, and the unique WLS solution is $x_{WLS} = [-3.8,\ 0.8,\ 8.6]^T$.

In the numerical computations, we use the MGS method with column pivoting, and take $d = 10^j$ with $j = 0,\ -2,\ -4,\ -6,\ -8,\ -10$.

Table 1.1. Numerical results for different j

j	0	-2	-4	-6	-8	-10
$\|\delta x_{WLS}\|$	1.78e-15	2.04e-14	2.14e-11	1.22e-6	2.01e-3	2.01e+1

From Table 1.1 we see that the ordinary MGS with column pivoting is numerically unstable, because $\mathrm{rank}(A(1:2,:)) = \mathrm{rank}(A(1:3,:)) = 2$, so with probability one, perturbed $\mathrm{rank}(\overline{A}(1:3,:)) = 3$ which violates the stability conditions in Eq. (3). Therefore, for this example the ordinary MGS with column pivoting is not enough for numerical stability in solving stiff WLS problem Eq. (1).

In this paper we will study situations similar to the above example, and propose a numerical stable row block MGS algorithm with column pivoting under Assumption 1.1.

The paper is organized as follows. In §2 we review some basic results for the ordinary MGS with column pivoting; in §3 we propose a numerical stable row block MGS algorithm with column pivoting for solving stiff WLS problem (1); in §4 we provide the roundoff error estimates of our new algorithm; in §5 numerical results of several examples are shown to verify the goodness of new algorithm and the roundoff error estimates in §4.

2. The MGS with Column Pivoting (PMGS)

In this section we first review some well-known results of the MGS with column pivoting (PMGS). The detailed description for the PMGS can be found in [9, 3, 7].

Suppose $A \in \Re_r^{m\times n}$, then the PMGS start with $A^{(1)} = A, R = O_n$, and then a sequence of matrices $A^{(2)}, \cdots, A^{(r+1)}$ will be computed, where $A^{(r+1)}(:, 1:r) = Q_1, A^{(r+1)}(:, r+1:n) = 0$ and $A^{(k)}$ has the form

$$A^{(k)}\Pi_k = [0, \cdots, 0, a_k^{(k)}, \cdots, a_n^{(k)}], \tag{4}$$

where the first $(k-1)$ columns of $A^{(k)}\Pi_k$ are generally used to store the known $q_1, \cdots, q_{k-1}$ for storage saving, Π_k is a permutation such that $\|a_k^{(k)}\| = \max_{j\geq k}\|a_j^{(k)}\|$, then compute q_k as

$$r_{kk} = \|a_k^{(k)}\|, \quad q_k = a_k^{(k)}/r_{kk}, \tag{5}$$

and orthogonalize $a_j^{(k)}(j \geq k)$ against

$$r_{kj} = q_k^T a_j^{(k)}, \quad a_j^{(k+1)} = a_j^{(k)} - r_{kj}q_k,\ j = k+1, \cdots, n. \tag{6}$$

After r steps, with $\Pi = \Pi_1 \cdots \Pi_r, Q_1 = (q_1, \cdots, q_r), R_1 = R(1:r,:)$, we obtain the factorization $A\Pi = Q_1R_1$, and the columns of Q_1 are orthogonal by construction.

Björck and Paige [3, 4] pointed out that the PMGS of A is numerically and mathematically equivalent to performing a sequence of Householder transformations on $\begin{pmatrix} O_n \\ A\Pi \end{pmatrix}$. Denote

$$G^{(k)} = \begin{pmatrix} R^{(k)} \\ A^{(k)} \end{pmatrix}, \quad R^{(1)} = O_n,\ A^{(1)} = A\Pi.$$

Then the k-th step of MGS of $A\Pi$ is equivalent to the following Householder transform:

$$\begin{aligned} &G^{(k+1)} = P_kG^{(k)}, \quad P_k = I - v_kv_k^T, \\ &v_k = \begin{pmatrix} -e_k \\ q_k \end{pmatrix}, \quad q_k = \frac{a_k^{(k)}}{\|a_k^{(k)}\|}. \end{aligned} \tag{7}$$

Thus, after r steps, with $P = P_1P_2\cdots P_p, \Pi = \Pi_1\Pi_2\cdots\Pi_p$, we have the factorization

$$\begin{pmatrix} O_n \\ A\Pi \end{pmatrix} = P\begin{pmatrix} R \\ 0 \end{pmatrix},$$

where $R = \begin{pmatrix} R_1 \\ 0_{n-r} \end{pmatrix} \in \Re_r^{n\times n}$ is upper trapezoidal R-factor.

3. The Row Block PMGS Algorithm

Although the PMGS is row-wise stable, in general it is not numerically stable for solving the stiff WLS problem Eq. (1), as mentioned in §1 and Example 1.1. In order to ensure numerical stability of an algorithm for solving the stiff WLS problem, we need to keep

$$\text{rank}(\overline{C}_j) = \text{rank}(C_j), \quad \text{for } j = 1, 2, \cdots, k,$$

in the numerical computation. The following row block MGS algorithm with column pivoting (the RBPMGS algorithm) is stable for solving the stiff WLS problem (1).

Before presenting the RBPMGS algorithm, we first review the MMGS method, which is the slight modification of the ordinary MGS.

For $A \in \Re_n^{m\times n}$ and $A^{(1)} = A$, let $R = O_n$, then at the kth step of MMGS, compute

$$\begin{aligned} &r_{kk} = \|a_k^{(k)}\|_2, \quad q_k = a_k^{(k)}/r_{kk}, \quad r_{kj} = q_k^T a_j^{(k)}, \\ &a_{sj}^{(k+1)} = \left(a_{sj}^{(k)} \sum_{i\neq s} (a_{ik}^{(k)})^2 - a_{sk}^{(k)} \sum_{i\neq s} a_{ik}^{(k)} a_{ij}^{(k)} \right) / r_{kk}^2,\ s = 1:m, \end{aligned} \tag{8}$$

where the last equality is equivalent to the second equality of (6) in the accurate arithmetic.

Algorithm 3.1: RBPMGS Given matrix $A \in \Re^{m\times n}$, $b \in \Re^m$, and weighting matrix D satisfying Assumption 1.1, in which $\mathrm{rank}(C_j) = p_j$ for $j = 1, \cdots, k$. Choose tolerances $\eta_l > 0$ for $l = 1, 2, \cdots, k$.

- *Step 1.* Set $A := [A, b]$, take $C_1 = d_1 A_1$, evaluate the p_1 times PMGS of C_1:

$$R^{(1)} := [\ R_{11}^{(1)} \quad R_{12}^{(1)}\ ] = [Q_1^{(1)}]^T C_1 \Pi^{(1)},$$
$$C_1^{(p_1+1)} := (Q_1^{(1)}, C_{12}^{(p_1+1)}),$$

where

$$R^{(1)} \in \Re^{p_1\times(n+1)},\ Q_1^{(1)} \in \Re^{m_1\times p_1},\ [Q_1^{(1)}]^T Q_1^{(1)} = I_{p_1},$$

and $\Pi^{(1)}$ is a permutation matrix (do not permute the last column), such that

$$R_{11}^{(1)}(1,1) \geq R_{11}^{(1)}(2,2) \geq \cdots \geq R_{11}^{(1)}(p_1,p_1) > d_1\eta_1,$$
$$\|C_1^{(p_1+1)}(:,j)\| \leq d_1\eta_1, \quad j = p_1+1, \cdots, n.$$

Set $A := A\Pi^{(1)}$.

- *Step 2.* For $l = 2 : k$, set

$$C_l := \begin{pmatrix} R^{(l-1)} \\ d_l A_l \end{pmatrix} \begin{matrix} p_{l-1} \\ m_l \end{matrix}. \tag{9}$$

Perform p_{l-1} times MMGS without column pivoting on C_l :

$$\widetilde{R}_l := \begin{pmatrix} R_{11}^{(l)} & R_{12}^{(l)} \end{pmatrix} := [Q_1^{(l)}]^T C_l,$$
$$C_l^{(r_{l-1}+1)} := (Q_1^{(l)}, C_{l2}^{(r_{l-1}+1)}),$$

where

$$\widetilde{R}_l \in \Re^{p_{l-1}\times(n+1)},\ Q_1^{(l)} \in R^{(p_{l-1}+m_l)\times p_{l-1}},\ [Q_1^{(l)}]^T Q_1^{(l)} = I_{p_{l-1}}.$$

- Continue performing $p_l - p_{l-1}$ times PMGS on $C_{l2}^{(p_{l-1}+1)}$:

$$R_{22}^{(l)} := [Q_2^{(l)}]^T C_{l2}^{(r_{l-1}+1)} \Pi^{(l)},$$
$$C_l^{(r_l+1)} := (Q_1^{(l)}, Q_2^{(l)}, C_{l3}^{(r_l+1)}),$$

where

$$R_{22}^{(l)} \in \Re^{(p_l-p_{l-1})\times(n+1-p_{l-1})},\ Q_2^{(l)} \in R^{(p_{l-1}+m_l)\times(p_l-p_{l-1})},$$

and $[Q_2^{(l)}]^T Q_2^{(l)} = I_{p_l-p_{l-1}}$, $\Pi^{(l)}$ is a permutation matrix (do not permute the last column), such that

$$R_{22}^{(l)}(1,1) \geq R_{22}^{(l)}(2,2) \geq \cdots \geq R_{22}^{(l)}(p_l-p_{l-1}, p_l-p_{l-1}) > d_l\eta_l,$$
$$\|C_l^{(p_l+1)}(:,j)\| \leq d_l\eta_l, \quad j = p_l+1, \cdots, n.$$

Set

$$A := A\Pi^{(l)}, \qquad R^{(l)} := \begin{pmatrix} R_{11}^{(l)} & R_{12}^{(l)} \\ 0 & R_{22}^{(l)} \end{pmatrix} \begin{matrix} p_{l-1} \\ p_l - p_{l-1} \end{matrix}.$$

- If $l < k$ goto Step 2.

We give several remarks on Algorithm 3.1.

Remark 3.1. The tolerances η_l are chosen to correctly determine the numerical ranks of C_l for $l = 1, 2, \cdots, k$. We will explain in the next section how to choose proper η_l.

Remark 3.2. We assume that $d_1 \gg \cdots \gg d_k$, so from Lemma 4.1 in the next section, we see that

$$\|(C_l)_j^{(p_{i-1}+1)}\| = \alpha\|R^{(l-1)}(p_{i-1}+1 : p_i, j)\| = \alpha\|R^{(i)}(p_{i-1}+1 : p_i, j)\|$$

for $i = 1 : l-1$, where $\alpha \sim 1$. On the other hand,

$$R^{(i)}(p_{i-1}+1, p_{i-1}+1) \geq R^{(i)}(p_{i-1}+2, p_{i-1}+2) \geq \cdots \geq R^{(i)}(p_i, p_i),$$

and therefore in the Step 2 of Algorithm 3.1, there is no need to interchange columns during the first p_{l-1} times MMGS method.

Remark 3.3. After performing Algorithm 3.1, we obtain a linear system of consistent equations

$$R^{(k)}(:, 1 : n)\Pi^T(:, 1 : n)x = R^{(k)}(:, n+1),$$

where $\Pi = \Pi^{(1)} \cdots \Pi^{(k)}$ and when $r = n$, $R^{(k)}(:, 1 : n)$ is upper-triangular and nonsingular; when $r < n$, $R^{(k)}(:, 1 : n)$ is upper-trapezoidal and has full row rank r. There are standard algorithms to solve the above system, see, e.g., [7]. Here we omit the details.

4. The Roundoff Error Analysis for Algorithm 3.1

In this section we provide the roundoff error estimates for Algorithm 3.1. We show that if the number of row blocks k is not too large, then with properly chosen tolerances η_l, Algorithm 3.1 is backward row-wise stable and can correctly determine the numerical ranks of C_l for $l = 1, \cdots, k$.

4.1. Notation

Let $D = W^{\frac{1}{2}} = \mathrm{diag}(d_1 I_{m_1}, d_2 I_{m_2}, \cdots, d_k I_{m_k})$, $\epsilon_{il} = (d_i/d_l)^2 \ll 1$ for $i > l$ and A, C_j, b take forms as in Assumption 1.1. Let $m = m_1 + m_2 + \cdots + m_k, p_0 \equiv 0, \mathrm{rank}(C_j) = p_j$, $j = 1, \cdots, k$.

Suppose that Π is the permutation matrix taking account of the overall column interchanges during the RBPMGS algorithm of DA. Denote

$$A^{(1)} = A\Pi \equiv \begin{pmatrix} A_1^{(1)} \\ \vdots \\ A_k^{(1)} \end{pmatrix} \begin{matrix} m_1 \\ \vdots \\ m_k \end{matrix} \qquad b = \begin{pmatrix} b_1 \\ \vdots \\ b_k \end{pmatrix} \qquad C_j^{(1)} = \begin{pmatrix} A_1^{(1)} \\ \vdots \\ A_j^{(1)} \end{pmatrix}, \quad j = 1 : k. \tag{10}$$

Let $(R_{[0]}^d, z_{[0]}^d)$ be a null matrix, and

$$\begin{aligned} &\begin{pmatrix} Y_{[\ell]}^{(1)} & w_{[\ell]}^{(1)} \end{pmatrix} \equiv \begin{pmatrix} O_n & 0 \\ \Gamma_{[\ell]}^{(1)} & g_{[\ell]}^{(1)} \end{pmatrix} = \begin{pmatrix} O_n & 0 \\ R_{[\ell-1]}^d & z_{[\ell-1]}^d \\ d_\ell A_\ell^{(1)} & d_\ell b_\ell \end{pmatrix}, \\ &\begin{pmatrix} Y_{[\ell]}^{(t+1)} & w_{[\ell]}^{(t+1)} \end{pmatrix} \equiv \begin{pmatrix} R_{[\ell]}^{d^{(t+1)}} & z_{[\ell]}^{d^{(t+1)}} \\ \Gamma_{[\ell]}^{(t+1)} & g_{[\ell]}^{(t+1)} \end{pmatrix} = \begin{pmatrix} R_{[\ell]}^{d^{(t+1)}} & z_{[\ell]}^{d^{(t+1)}} \\ R_{[\ell-1]}^{d^{(t+1)}} & z_{[\ell-1]}^{d^{(t+1)}} \\ d_\ell A_\ell^{(t+1)} & d_\ell b_\ell^{(t+1)} \end{pmatrix}, \\ &[R_{[\ell]}^{d^{(t+1)}}, z_{[\ell]}^{d^{(t+1)}}] \in \Re_t^{n\times(n+1)}, \quad \Gamma_{[\ell]}^{(t+1)}(:, 1 : t) = 0, \quad 1 \leq t \leq p_\ell, \end{aligned} \tag{11}$$

for $\ell = 1, \cdots, k$, where $[Y_{[\ell]}^{(t+1)}, w_{[\ell]}^{(t+1)}]$ is accurately computed from $[Y_{[\ell]}^{(1)}, w_{[\ell]}^{(1)}]$ via $\min\{t, p_{\ell-1}\}$ times MMGS and $\max\{t - p_{\ell-1}, 0\}$ times MGS of $[\Gamma_{[\ell]}^{(1)}, g_{[\ell]}^{(1)}]$, and $[R_{[\ell]}^d, z_{[\ell]}^d] \equiv [R_{[\ell]}^{d^{(p_\ell+1)}}, z_{[\ell]}^{d^{(p_\ell+1)}}] \in \Re_{p_\ell}^{n\times(n+1)}$ is the corresponding upper trapezoidal R–factor taking the form

$$\left(R_{[\ell]}^d, z_{[\ell]}^d\right) \equiv D_{[\ell]}\left(R_{[\ell]}, z_{[\ell]}\right) = \begin{pmatrix} d_1 R_{[\ell]}^{1,1} & d_1 R_{[\ell]}^{1,2} & \cdots & d_1 R_{[\ell]}^{1,\ell} & d_1 z_{[\ell]}^1 \\ & d_2 R_{[\ell]}^{2,2} & \cdots & d_2 R_{[\ell]}^{2,\ell} & d_2 z_{[\ell]}^2 \\ & & \ddots & \vdots & \vdots \\ & \mathbf{0} & & d_\ell R_{[\ell]}^{\ell,\ell} & d_\ell z_{[\ell]}^\ell \\ & & & 0_{n-p_\ell} & 0 \end{pmatrix}, \tag{12}$$

where

$$D_{[\ell]} = \mathrm{diag}(d_1 I_{p_1}, \cdots, d_\ell I_{p_\ell - p_{\ell-1}}, I_{n-p_\ell}), \quad d_j R_{[\ell]}^{j,j} \in \Re^{(p_j - p_{j-1})\times(p_j-p_{j-1})}$$

are nonsingular.

Let $\overline{R}_{[\ell]}^d$, $\overline{R}_{[\ell]}$, $(\overline{\Gamma}_{[\ell]}^{(t)}, \overline{g}_{[\ell]}^{(t)})$, $\cdots$ be the computed versions of $R_{[\ell]}^d$, $R_{[\ell]}, (\Gamma_{[\ell]}^{(t)}, g_{[\ell]}^{(t)})$, $\cdots$. Write $\overline{R}_{[\ell]}^{(t)} \equiv ((\overline{R}_{[\ell]})_{ij}^{(t)}), \overline{\Gamma}_{[\ell]}^{(t)} \equiv ((\overline{\Gamma}_{[\ell]})_{ij}^{(t)})$. For $\ell = 1 : k, t = 1 : p_\ell, i = 1 : n_\ell + m_\ell$, where $n_1 = 0$, and $n_j = n$; otherwise, define

$$\begin{aligned}
&s_t^{(\ell)} = \max_{j\geq t} \|(\overline{\Gamma}_{[\ell]})_j^{(t)}\|_2, \quad \nu_t^{(\ell)} = \|\overline{g}_{[\ell]}^{(t)}\|_2, \\
&\alpha_i^{(\ell)} = \max_{1\leq t\leq p_\ell, j} |(\overline{\Gamma}_{[\ell]})_{ij}^{(t)}|, \quad \mu_i^{(\ell)} = \max_{1\leq t\leq p_\ell} |(\overline{g}_{[\ell]})_i^{(t)}|, \\
&S_\ell^{R_{[\ell]}^d} = \max_{i<t\leq p_\ell, j>t} \{|s_i^{R_{[\ell]}^d}(t,j)|\}, \\
&\zeta_c = \max\{1, \max_{1\leq\ell\leq k} \max_{1\leq t\leq p_\ell} (\nu_t^{(\ell)}/s_t^{\ell})\}, \\
&\zeta_r = \max\{1, \zeta_c, \max_{1\leq\ell\leq k} \max_{1\leq i\leq n_\ell+m_\ell} (\mu_i^{(\ell)}/\alpha_i^{(\ell)})\}, \\
&p_{[\ell]} = \prod_{i=2}^{\ell} p_i^{2.5}, \qquad \kappa_{[\ell]} = \prod_{i=2}^{\ell} S_i^{R_{[i]}^d}, \\
&\zeta_{[s,\,\ell]} = \max_{1\leq i\leq p_s, j\geq i} \|(A_\ell)_j^{(i)}\|_2, \qquad \Upsilon_{[\ell]} = \prod_{i=2}^{\ell} \max\{1, \frac{\zeta_{[i\,-\,1,\,i]}}{\min\limits_{1\leq s\leq p_{i-1}} (R_{[i\,-\,1]})_{ss}}\},
\end{aligned} \tag{13}$$

where the $s_i^{R_{[l]}^d}(t,j)$ satisfy

$$\begin{aligned}
&s_0^{R_{[l]}^d}(t,j) = 1, \quad s_1^{R_{[l]}^d}(t,j) = \frac{(R_{[l]}^d)_{tj}}{(R_{[l]}^d)_{tt}}, \\
&s_i^{R_{[k]}^d}(t,j) = \frac{\det((R_{[l]}^d)(t+1-i:k, t+2-i:t; j))}{\prod\limits_{h=0}^{i-1} (R_{[l]}^d)_{t-h,t-h}}, \quad i = 2:k.
\end{aligned}$$

Furthermore, we assume

$$\sum_{i=s}^{t} h(i) = 0, \quad \prod_{i=s}^{t} h(i) = 1, \quad \text{if } s > t,$$

where $h(i)$ is an expression in i.

Remark 4.1. In (13), $S_l^{R_{[l]}^d}$ can be replaced by $S_l^{R_{[l]}}$, since $v_{t-i+1} = (-1)^{i-1} s_i^{R_{[l]}^d}(t,j)$, for $i = 1 : t$ solve the equation: $R_{[l]}^d(1:t, 1:t)v = R_{[l]}^d(1:t, j)$. Pre-multiplying $D_{[l]}^{-1}$ on the two sides of the equality yields

$$R_{[l]}(1:t,1:t)v = R_{[l]}(1:t,j),$$

which is equivalent to $s_i^{R^d_{[l]}}(t,j) = s_i^{R_{[l]}}(t,j)$.

Remark 4.2. When the number of row blocks k is not too large, then we see from Theorem 4.1 that the computed $\overline{R}_{[l]}$ contains small roundoff errors, and

$$(R_{[l]})^2_{hh} \gtrsim \sum_{i=h}^{\min\{p_{t-1}+1,p_t\}} (R_{[l]})^2_{ij}, \qquad 1 \le h \le p_l, \quad j \ge h,$$

where t is an integer satisfying $p_{t-1} < h \le p_t$; thus $s_i^{R^d_{[l]}}(t,j)$ are generally of unit order, as mentioned in [20].

4.2. The forward roundoff errors of the RBPMGS algorithm

We first discuss the forward roundoff errors of the RBPMGS algorithm. We have studied the forward roundoff errors of the PMGS for a single matrix A_1 in [20]. From now on we assume that $k \ge 2$ in Assumption 1.1.

The following lemma explains why the MMGS is needed in the RBPMGS algorithm.

Lemma 4.1. *Let* $\epsilon_{21} = (d_2/d_1)^2$, $R^d_{[1]} \equiv d_1 R_{[1]} \in \Re^{n\times n}_{p_1}, \Gamma^{(1)}_{[2]}$ *be defined as* (11), *and*

$$\begin{aligned} Y^{(p_1+1)} &= P^{(2)}_{p_1} \cdots P^{(2)}_2 P^{(2)}_1 Y^{(1)} \\ &= \begin{pmatrix} R^{d^{(p_1+1)}}_{[2]} \\ \Gamma^{(p_1+1)}_{[2]} \end{pmatrix} \equiv \begin{pmatrix} d_1 R^{(p_1+1)}_{[2]} \\ d_1 R^{(p_1+1)}_{[1]} \\ d_2 (A_2)^{(p_1+1)} \end{pmatrix} \end{aligned}$$

be obtained from $Y^{(1)} = \begin{pmatrix} 0_n \\ \Gamma^{(1)}_{[2]} \end{pmatrix}$ *via* p_1 *times accurate MGS without column pivoting. Then for* $l = 1, \cdots, p_1$,

$$\begin{aligned} &\|(R_{[2]})^{(p_1+1)}_j\|_2 = \|(R_{[1]})_j\|_2(1+\mathcal{O}(\epsilon_{21})), \;\; j = 1:n; \\ &(R_{[2]})^{(p_1+1)}_{lh} = (R_{[1]})_{lh}(1+\mathcal{O}(\epsilon_{21})), \;\; h \ge l; \\ &(R_{[1]})^{(l+1)}_{ij} = \mathcal{O}(\epsilon_{21}), \;\; i \le l, j \ge l+1; \\ &(A_2)^{(l+1)}_j = (A_2)^{(l)}_j - \frac{(R_{[1]})_{lj}}{(R_{[1]})_{ll}}(1+\mathcal{O}(\epsilon_{21}))(A_2)^{(l)}_l \\ &\qquad = \cdots \\ &\qquad = (A_2)^{(1)}_j - \sum_{h=1}^{l} \frac{(R_{[1]})_{hj}}{(R_{[1]})_{hh}}(1+\mathcal{O}(\epsilon_{21}))(A_2)^{(h)}_h. \end{aligned} \tag{14}$$

Proof. Using the invariance of the 2-norm under orthogonal transformations, we obtain

$$\begin{aligned} d_1\|(R_{[2]})^{(p_1+1)}_j\|_2 &= d_1\|(R_{[2]})^{(j+1)}_j\|_2 \\ &= \|(\Gamma_{[2]})^{(1)}_j\|_2 = d_1\|(R_{[1]})_j\|_2(1+\mathcal{O}(\epsilon_{21})). \end{aligned}$$

We now prove the remaining part of (14). When $l = 1$, then for $j = 2, \cdots, n$, we have

$$\begin{aligned} & d_1(R_{[2]})_{1h}^{(p_1+1)} = \frac{(\Gamma_{[2]})_1^{(1)^T}(\Gamma_{[2]})_h^{(1)}}{\|(\Gamma_{[2]})_1^{(1)}\|_2} \\ = & \frac{d_1^2(R_{[1]})_{11}(R_{[1]})_{1h} + d_2^2(A_2)_1^{(1)^T}(A_2)_h^{(1)}}{(d_1^2(R_{[1]})_{11}^2 + d_2^2\|(A_2)_1^{(1)}\|_2^2)^{\frac{1}{2}}} \\ = & \frac{d_1^2(R_{[1]})_{11}(R_{[1]})_{1h}(1+\mathcal{O}(\epsilon_{21}))}{d_1(R_{[1]})_{11}(1+\mathcal{O}(\epsilon_{21}))} \\ = & d_1(R_{[1]})_{1h}(1+\mathcal{O}(\epsilon_{21})), \end{aligned}$$

$$\begin{aligned} & d_1(R_{[1]})_{1j}^{(2)} = (\Gamma_{[2]})_{1j}^{(2)} \\ = & (\Gamma_{[2]})_{1j}^{(1)} - \frac{(\Gamma_{[2]})_1^{(1)^T}(\Gamma_{[2]})_j^{(1)}}{\|(\Gamma_{[2]})_1^{(1)}\|_2^2}(\Gamma_{[2]})_{11}^{(1)} \\ = & \frac{d_1 d_2^2\left((R_{[1]})_{1j}\|(A_2)_1^{(1)}\|_2^2 - (R_{[1]})_{11}(A_2)_1^{(1)^T}(A_2)_j^{(1)}\right)}{d_1^2(R_{[1]})_{11}^2 + d_2^2\|(A_2)_1^{(1)}\|_2^2} \\ = & d_1\epsilon_{21}\frac{(R_{[1]})_{1j}\|(A_2)_1^{(1)}\|_2^2 - (R_{[1]})_{11}(A_2)_1^{(1)^T}(A_2)_j^{(1)}}{(R_{[1]})_{11}^2}(1+\mathcal{O}(\epsilon_{21})) \\ = & \mathcal{O}(d_1\epsilon_{21}), \end{aligned}$$

and

$$\begin{aligned} & d_2(A_2)_j^{(2)} = d_2(A_2)_j^{(1)} - \frac{d_1^2(R_{[1]})_{11}(R_{[1]})_{1j} + d_2^2(A_2)_1^{(1)^T}(A_2)_j^{(1)}}{d_1^2(R_{[1]})_{11}^2 + d_2^2\|(A_2)_1^{(1)}\|_2^2}d_2(A_2)_1^{(1)} \\ = & d_2(A_2)_j^{(1)} - d_2\frac{(R_{[1]})_{1j}}{(R_{[1]})_{11}}(1+\mathcal{O}(\epsilon_{21}))(A_2)_1^{(1)}. \end{aligned}$$

Thus (14) holds for $l = 1$. Assume that (14) holds for $1 \le l < s$. Then for $l = s$, we obtain

$$(\Gamma_{[2]})_h^{(s)} = \begin{pmatrix} d_1(R_{[1]})_h^{(s)} \\ d_2(A_2)_h^{(s)} \end{pmatrix}, \quad h \ge s,$$

where

$$(R_{[1]})_h^{(s)} = ((R_{[1]})_{1h}^{(s)}, \cdots, (R_{[1]})_{s-1,h}^{(s)}, (R_{[1]})_{sh}^{(s)}, \cdots, (R_{[1]})_{hh}^{(s)}, 0, \cdots, 0)^T,$$

and $(R_{[1]})_{is}^{(s)} = \mathcal{O}(\epsilon_{21})$, $i = 1, \cdots, s-1$ by assumption; and for $i \ge s$ and all j, $(R_{[1]})_{ij}^{(s)} = (R_{[1]})_{ij}$ since $R_{[1]}$ is upper trapezoidal. Thus

$$\begin{aligned} & d_1(R_{[2]})_{sh}^{(p_1+1)} = \frac{(\Gamma_{[2]})_s^{(s)^T}(\Gamma_{[2]})_h^{(s)}}{\|(\Gamma_{[2]})_s^{(s)}\|_2} \\ = & \frac{\mathcal{O}(d_2^2\epsilon_{21}) + d_1^2(R_{[1]})_{ss}(R_{[1]})_{sh} + d_2^2(A_2)_s^{(s)^T}(A_2)_h^{(s)}}{(\mathcal{O}(d_2^2\epsilon_{21}) + d_1^2(R_{[1]})_{ss}^2 + d_2^2\|(A_2)_s^{(s)}\|_2^2)^{\frac{1}{2}}} \\ = & d_1(R_{[1]})_{sh}(1+\mathcal{O}(\epsilon_{21})), \end{aligned}$$

and for $i < s$, $j \geq s+1$,

$$d_1(R_{[1]})_{ij}^{(s+1)} = (\Gamma_{[2]})_{ij}^{(s+1)} = (\Gamma_{[2]})_{ij}^{(s)} - \frac{(\Gamma_{[2]})_s^{(s)^T}(\Gamma_{[2]})_j^{(s)}}{\|(\Gamma_{[2]})_s^{(s)}\|_2^2}(\Gamma_{[2]})_{is}^{(s)} = \mathcal{O}(d_1\epsilon_{21}),$$

$$\begin{aligned}
d_1(R_{[1]})_{sj}^{(s+1)} &= (\Gamma_{[2]})_{sj}^{(s+1)} = (\Gamma_{[2]})_{sj}^{(s)} - \frac{(\Gamma_{[2]})_s^{(s)^T}(\Gamma_{[2]})_j^{(s)}}{\|(\Gamma_{[2]})_s^{(s)}\|_2^2}(\Gamma_{[2]})_{ss}^{(s)} \\
&= \frac{d_1 d_2^2\{(R_{[1]})_{sj}^{(s)}\|(A_2^{(s)})_s\|_2^2 - (R_{[1]})_{ss}^{(s)}(A_2)_s^{(s)^T}(A_2)_j^{(s)}\} + \mathcal{O}(d_1 d_2^2\epsilon_{21})}{d_1^2(R_{[1]})_{ss}^{(s)^2} + d_2^2\|(A_2)_s^{(s)}\|_2^2 + \mathcal{O}(d_2^2\epsilon_{21})} \\
&= d_1\epsilon_{21}\frac{(R_{[1]})_{sj}\|(A_2)_s^{(s)}\|_2^2 - (R_{[1]})_{ss}(A_2)_s^{(s)^T}(A_2)_j^{(s)}}{(R_{[1]})_{ss}^2}(1+\mathcal{O}(\epsilon_{21})) = \mathcal{O}(d_1\epsilon_{21}),
\end{aligned}$$

$$\begin{aligned}
d_2(A_2)_j^{(s+1)} &= d_2(A_2)_j^{(s)} - \frac{\mathcal{O}(d_2^2\epsilon_{21}) + d_1^2(R_{[1]})_{ss}(R_{[1]})_{sj} + d_2^2(A_2)_s^{(s)^T}(A_2)_j^{(s)}}{\mathcal{O}(d_2^2\epsilon_{21}) + d_1^2(R_{[1]})_{ss}^2 + d_2^2\|(A_2)_s^{(s)}\|_2^2}d_2(A_2)_s^{(s)} \\
&= d_2(A_2)_j^{(s)} - d_2\frac{(R_{[1]})_{sj}}{(R_{[1]})_{ss}}(1+\mathcal{O}(\epsilon_{21}))(A_2)_s^{(s)} \\
&= d_2(A_2)_j^{(1)} - d_2\sum_{h=1}^{s}\frac{(R_{[1]})_{hj}}{(R_{[1]})_{hh}}(1+\mathcal{O}(\epsilon_{21}))(A_2)_h^{(h)}.
\end{aligned}$$

Thus (14) holds for $l = s$. By induction, we see that (14) holds for $l = 1, 2, \cdots, p_1$.

From Lemma 4.1 we see that, when

$$d_2 \ll d_1,\ 1 \leq l \leq p_1,\ \ q_l = (\Gamma_{[2]})_l^{(l)}/\|(\Gamma_{[2]})_l^{(l)}\|_2 \sim e_l,$$

and therefore if we orthogonalize $(\Gamma_{[2]})_j^{(l+1)}$ against q_l during the floating point arithmetic of the MGS, then cancellation will arise in the computation of $(\Gamma_{[2]})_{lj}^{(l+1)}$, and reduces the significant digits of $(\Gamma_{[2]})_{lj}^{(l+1)}$. We can avoid this by the MMGS method.

Using the same technique as in Lemma 4.1, we can prove the following lemma.

Lemma 4.2. *Let* $\epsilon_{il} = (d_i/d_l)^2 \ll 1$ *for* $i > l$, *and*

$$\Gamma_{[\ell]}^{(1)} = \begin{pmatrix} R_{[\ell-1]}^d \\ d_\ell A_\ell^{(1)} \end{pmatrix}$$

be defined as (11), *where*

$$R_{[\ell-1]}^d = D_{[\ell-1]}R_{[\ell-1]}$$

takes the form of (12). *Suppose that* $R_{[\ell]}^d \equiv D_{[k]}R_{[\ell]}$ *is the upper trapezoidal R–factor accurately computed from* $\Gamma_{[\ell]}^{(1)}$ *via* $p_{\ell-1}$ *times MMGS and* $p_\ell - p_{\ell-1}$ *times MGS. Set*

$$\begin{aligned}
&q_t = \frac{(\Gamma_{[\ell]})_t^{(t)}}{\|(\Gamma_{[\ell]})_t^{(t)}\|_2}, \quad M_t = I - q_t q_t^T, \quad t = 1 : p_{\ell-1}, \\
&\Gamma_{[\ell]}^{(p_{h-1}+t_h)} = M_{p_{h-1}+t_h-1}\cdots M_2 M_1 \Gamma_{[\ell]}^{(1)},
\end{aligned}$$

for $h = 1 : \ell - 1, t_h = 1 : p_h - p_{h-1}$. *Then*

$$(\Gamma_{[\ell]})_{ij}^{(p_{h-1}+t_h)} = \begin{cases} \mathcal{O}(d_s\epsilon_{\ell,s}), \quad 1 \le i < p_{h-1}+t_h, \quad \exists\, 1 \le s \le h & s.t. \;\; p_{s-1} < i \le p_s, \\ (R^d_{[\ell-1]})_{ij}, & p_{h-1}+t_h \le i \le p_{\ell-1}, \\ 0, & p_{\ell-1} < i \le n, \\ -d_\ell \displaystyle\sum_{l=1}^{p_{h-1}+t_h-1} \frac{\beta_l^\ell (R_{[\ell-1]})_{lj}}{(R_{[\ell-1]})_{ll}} (A_\ell)_{il}^{(l)}, & n < i \le n+m_\ell. \end{cases} \tag{15}$$

where $\beta_l^\ell = 1 + \mathcal{O}(\epsilon_{\ell,s})$, *and* s *is an integer satisfying* $p_{s-1} < l \le p_s$. *Moreover,*

$$(R_{[\ell]})_{p_{h-1}+t_h,l} = \alpha(R_{[\ell-1]})_{p_{h-1}+t_h,l} = \cdots = \alpha(R_{[h]})_{p_{h-1}+t_h,l}, \quad \alpha \sim 1, \tag{16}$$

for $l \ge p_{h-1}+t_h$, *and if we let*

$$z^{(1)} = D_{[\ell-1]}\eta^{(1)}, \qquad z^{(p_{h-1}+t_h)} = M_{p_{h-1}+t_h-1}\cdots M_1 z^{(1)},$$

where $\eta_i^{(1)} \sim \mathbf{u}$, *for* $i = 1 : p_{\ell-1}$; *and* $\eta_i^{(1)} = 0$ *otherwise, then*

$$z_i^{(p_{h-1}+t_h)} = \begin{cases} \mathcal{O}(d_s\epsilon_{\ell,s}), & 1 \le i < p_{h-1}+t_h, \quad \exists\, 1 \le s \le h \quad s.t. \;\; p_{s-1} < i \le p_s, \\ z_i^{(1)}, & p_{h-1}+t_h \le i \le p_{\ell-1}, \\ 0, & p_{\ell-1} < i \le n, \\ -d_\ell \displaystyle\sum_{l=1}^{p_{h-1}+t_h-1} \frac{\beta_l^\ell \eta_l^{(1)}}{(R_{[\ell-1]})_{ll}} (A_\ell)_{il}^{(l)}, & n < i \le n+m_\ell. \end{cases} \tag{17}$$

Based on the above lemmas, we now study the forward roundoff errors of the RBPMGS algorithm.

Theorem 4.1. *Define* $j_h = \min\{j, h\}$, *and under the notations in* (10)–(13) *consider the RBPMGS of* $(DA^{(1)}, Db)$ *without column pivoting. If*

$$\begin{aligned} &\widetilde{\gamma}_m \phi_{p_1}^{(1)} (R_{[1]})_{11} \ll (R_{[1]})_{p_1,p_1}, \\ &\widetilde{\gamma}_m \widetilde{\phi}^{(\ell)}_{p_\ell - p_{\ell-1},\ell} \max_{1\le i\le p_\ell, j\ge i} |(R_{[\ell]})_{ij}| \ll (R_{[\ell]})_{p_\ell,p_\ell}, \quad for \quad \ell = 2 : k, \end{aligned}$$

then we have the following estimates:

$$\begin{aligned} &|(\overline{R}_{[\ell]})_{p_{h-1}+t_h,j} - (R_{[\ell]})_{p_{h-1}+t_h,j}| \le \widetilde{\gamma}_m \widetilde{\phi}^{(h)}_{t_h,\ell} \max_{1\le i\le p_h, j\ge i} |(R_{[\ell]})_{ij}|, \\ &\|(\overline{\Gamma}_{[\ell]})_j^{(p_{h-1}+t_h)} - (\Gamma_{[\ell]})_j^{(p_{h-1}+t_h)}\|_2 \le d_h \widetilde{\gamma}_m \widetilde{\phi}^{(h)}_{t_h,\ell} \max_{1\le i\le p_h, j\ge i} |(R_{[\ell]})_{ij}|, \\ &|(\overline{z}_{[\ell]})_{p_{h-1}+t_h,j} - (z_{[\ell]})_{p_{h-1}+t_h,j}| \le \widetilde{\gamma}_m \widetilde{\phi}^{(h)}_{t_h,\ell} \zeta_c \max_{1\le i\le p_h, j\ge i} |(R_{[\ell]})_{ij}|, \\ &\|(\overline{g}_{[\ell]})^{(p_{h-1}+t_h)} - (g_{[\ell]})^{(p_{h-1}+t_h)}\|_2 \le d_h \widetilde{\gamma}_m \widetilde{\phi}^{(h)}_{t_h,\ell} \zeta_c \max_{1\le i\le p_h, j\ge i} |(R_{[\ell]})_{ij}|, \end{aligned} \tag{18}$$

for $h = 1 : \ell$, *and* $t_h = 1 : \delta_{h,\ell} + p_h - p_{h-1}$, *where* $\delta_{h,\ell} = 1$ *for* $h = \ell$; $\delta_{h,\ell} = 0$ *otherwise, and*

$$\widetilde{\phi}^{(h)}_{s,\ell} = \begin{cases} (j_{p_h} - p_{h-1} - s + 1)^{0.5} (j_{p_h} - p_{h-1})^{0.5(\ell-h-1)} p_{[h]} \Upsilon_{[h]} \kappa_{[h]} \phi^{(1)}_{p_1}, & h = 1 : \ell - 1, \\ (p_{\ell-1} + s)^{2.5} p_{[\ell-1]} \Upsilon_{[\ell]} \kappa_{[\ell]} \phi^{(1)}_{p_1}, & h = \ell, \end{cases}$$

where

$$\phi_1^{(1)} = 1, \phi_l^{(1)} = \min\{S_1^{R_{[1]}} l^{2.5}, 2^l - 1\} \;\; for \;\; 2 \le l \le p_1.$$

Proof. Since the proof is lengthy, we outline the proof in the following steps.
Step 1. For $l = 1 : p_\ell, j = l : n$, let

$$(\xi_{[\ell]})_j^{(l)} \equiv (\overline{\Gamma}_{[\ell]})_j^{(l)} - (\Gamma_{[\ell]})_j^{(l)}, \quad M_l = I - q_l q_l^T, \quad \widehat{M}_l = I - \widehat{q}_l \widehat{q}_l^T,$$

where

$$q_l = (\Gamma_{[\ell]})_l^{(l)} / \|(\Gamma_{[\ell]})_l^{(l)}\|_2, \widehat{q}_l = (\overline{\Gamma}_{[\ell]})_l^{(l)} / \|(\overline{\Gamma}_{[\ell]})_l^{(l)}\|_2.$$

Then $(\xi_{[\ell]})_j^{(1)}$ takes the form

$$(\xi_{[\ell]})_j^{(1)} = \begin{pmatrix} (\delta R^d_{[\ell-1]})_j \\ 0_{m_\ell} \end{pmatrix} \equiv \begin{pmatrix} D_{[\ell-1]}(\delta R_{[\ell-1]})_j \\ 0_{m_\ell} \end{pmatrix},$$

where

$$\delta R^d_{[\ell-1]} = \overline{R}^d_{[\ell-1]} - R^d_{[\ell-1]},$$

with the last $n - p_{\ell-1}$ rows zero. Consequently,

$$\|(\xi_{[\ell]})_j^{(1)}\|_2 \le d_1 j_{p_1}^{0.5} \max_{1 \le s \le p_1} |(\delta R_{[\ell-1]})_{sj}|, \tag{19}$$

since $d_i \ll d_1$ for $i > 1$.

Because the first $p_{\ell-1}$ transformations performed on $\overline{\Gamma}_{[\ell]}^{(1)}$ are the MMGS method, and the last $p_\ell - p_{\ell-1}$ times transformations are the MGS method, we then derive from the standard roundoff error estimates that

$$(\overline{\Gamma}_{[\ell]})_j^{(p_{h-1}+t_h+1)} = \widehat{M}_{p_{h-1}+t_h} (\overline{\Gamma}_{[\ell]})_j^{(p_{h-1}+t_h)} + (\overline{\delta}_{[\ell]})_j^{(p_{h-1}+t_h)}, \tag{20}$$

holds for

(i) $1 \le h \le \ell - 1, 1 \le t_h \le p_h - p_{h-1}$, i.e. during the MMGS method:

$$|(\overline{\delta}_{[\ell]})_j^{(p_{h-1}+t_h)}| \le \widetilde{\gamma}_m \begin{pmatrix} \mathcal{O}(d_1 \epsilon_{\ell,1}) \\ \vdots \\ \mathcal{O}(d_{h-1} \epsilon_{\ell,h-1}) \\ \mathcal{O}(d_h \epsilon_{\ell,h}) \\ 0 \\ d_\ell (|(A_\ell)_{p_{h-1}+t_h}^{(p_{h-1}+t_h)}| + |(A_\ell)_j^{(p_{h-1}+t_h)}|) \end{pmatrix} \begin{matrix} p_1 \\ \vdots \\ p_{h-1} - p_{h-2} \\ t_h \\ n - p_{h-1} - t_h \\ m_\ell \end{matrix}$$

which is equivalent to

$$\|(\overline{\delta}_{[\ell]})_j^{(p_{h-1}+t_h)}\|_2 \le d_\ell \widetilde{\gamma}_m \max_{j \ge p_{h-1}+t_h} \|(A_\ell)_j^{(p_{h-1}+t_h)}\|_2 + \mathcal{O}(d_\ell \epsilon_{\ell,h}^{\frac{1}{2}} \widetilde{\gamma}_m). \tag{21}$$

(ii) $h = \ell, 1 \le t_\ell \le p_\ell - p_{\ell-1} + 1$, i.e. during the MGS method:

$$\|(\overline{\delta}_{[\ell]})_j^{(p_{\ell-1}+t_\ell)}\|_2 \le \widetilde{\gamma}_m \|(\overline{\Gamma}_{[\ell]})_{p_{\ell-1}+1}^{(p_{\ell-1}+1)}\|_2 \le d_\ell \widetilde{\gamma}_m (R_{[\ell]})_{p_{\ell-1}+1, p_{\ell-1}+1}. \tag{22}$$

From the formula in [20], we see that the $(\xi_{[\ell]})_j^{(l+1)}$ satisfy

$$\begin{aligned} (\xi_{[\ell]})_j^{(l+1)} &= M_l (\xi_{[\ell]})_j^{(l)} + [M_l (\xi_{[\ell]})_l^{(l)} q_l^T + q_l (\xi_{[\ell]})_l^{(l)T} M_l] \frac{-(\Gamma_{[\ell]})_j^{(l)}}{\|(\Gamma_{[\ell]})_l^{(l)}\|_2} + (\delta_{[\ell]})_j^{(l)} \\ &= \Delta_j^{(l)} + \sum_{i=1}^{l-1} \Psi_{j,l}^{(i)} (\Delta_{l-i+1}^{(l-i)}), \quad l \ge 2, \end{aligned} \tag{23}$$

where

$$\Delta_j^{(1)} = (\delta_{[\ell]})_j^{(1)} = (\xi_{[\ell]})_j^{(2)}; \quad \Delta_j^{(s)} = (\delta_{[\ell]})_j^{(s)} + \sum_{i=1}^{s-1} M_s \cdots M_{i+1} (\delta_{[\ell]})_j^{(i)}$$

for $s \geq 2$, and

$$\begin{aligned} (\delta_{[\ell]})_j^{(1)} &= M_1(\xi_{[\ell]})_j^{(1)} + (M_1(\xi_{[\ell]})_1^{(1)} q_1^T + q_1 (\xi_{[\ell]})_1^{(1)^T} M_1) \frac{-(\Gamma_{[\ell]})_j^{(1)}}{\|(\Gamma_{[\ell]})_1^{(1)}\|_2} \\ &\quad + (\overline{\delta}_{[\ell]})_j^{(1)} + \alpha(\|(\xi_{[\ell]})_j^{(1)}\|_2^2 + \|(\xi_{[\ell]})_1^{(1)}\|_2^2), \quad \alpha \sim 1, \\ (\delta_{[\ell]})_j^{(s)} &= (\overline{\delta}_{[\ell]})_j^{(s)} + \alpha(\|(\xi_{[\ell]})_s^{(s)}\|_2^2 + \|(\xi_{[\ell]})_j^{(s)})\|_2^2), \ 2 \leq s \leq p_\ell, \\ \Psi_{j,l}^{(i)}(x) &= (-1)^i s_i^{R_{[\ell]}^d}(l,j)(\prod_{t=0}^{i-1} M_{l-t})x + \\ &\quad + \sum_{t=0}^{i-1} \frac{(\Gamma_{[\ell]})_j^{(l+1)T}(\prod_{t=0}^{i-1} M_{l-t})x}{(R_{[\ell]}^d)_{l-t,l-t}} (-1)^{i-t} s_{i-1-t}^{R_{[\ell]}^d}(l-1-t, l-t) q_{l-t}. \end{aligned} \tag{24}$$

Step 2. Using (23)–(24) to derive the formula bounding $\|(\xi_{[\ell]})_j^{(p_{h-1}+t_h)}\|_2$, for $h = 1 : \ell - 1, t_h = 1 : p_h - p_{h-1}, j \geq p_{h-1} + t_h$.

By (23)-(24), and setting $h = 1, \ t_h = 2$ in (17), we obtain

$$\begin{aligned} \|(\xi_{[\ell]})_j^{(2)}\|_2 &= \|\Delta_j^{(1)}\|_2 \leq \|M_1(\xi_{[\ell]})_j^{(1)}\|_2 + \beta_j \|M_1(\xi_{[\ell]})_1^{(1)}\|_2 + \|(\overline{\delta}_{[\ell]})_j^{(1)}\|_2 \\ &= \|M_1(\xi_{[\ell]})_j^{(1)}\|_2(1 + \mathcal{O}(\epsilon_{\ell,1}^{\frac{1}{2}})) \\ &\leq d_1(j_{p_1} - 1)^{0.5} \alpha \max_{1 \leq s \leq p_1} (\delta R_{[\ell-1]})_{sj}|, \quad \alpha \sim 1, \end{aligned} \tag{25}$$

where

$$\beta_j = \frac{\|(\Gamma_{[\ell]})_j^{(1)}\|_2}{\|(\Gamma_{[\ell]})_1^{(1)}\|_2} = \beta \frac{\|(R_{[\ell-1]}^d)_j\|_2}{\|(R_{[\ell-1]}^d)_1\|_2} = \beta \frac{\|(R_{[1]}^d)_j\|_2}{\|(R_{[1]}^d)_1\|_2} \leq \beta, \quad \beta \sim 1.$$

When $l = p_{h-1} + t_h - 1 \geq 2$, note from (17),(21) and (24) that for $j \geq l + 1$,

$$\begin{aligned} \|M_l \cdots M_2(\delta_{[\ell]})_j^{(1)}\|_2 \quad &\leq \|M_l \cdots M_2(\xi_{[\ell]})_j^{(1)}\|_2 + \beta_j \|M_1(\xi_{[\ell]})_1^{(1)}\|_2 + \|(\overline{\delta}_{[\ell]})_j^{(1)}\|_2 \\ &\leq d_h(j_{p_h} - p_{h-1} - t_h + 1)^{0.5} \alpha \max_{p_{h-1} < s \leq p_h} |(\delta R_{[\ell-1]})_{sj}|, \end{aligned}$$

and for $2 \leq s \leq l$, $\|M_l \cdots M_2(\delta_{[\ell]})_s^{(1)}\|_2 \sim \mathcal{O}(d_\ell \widetilde{\gamma}_m)$. Consequently,

$$\begin{aligned} \|\Delta_j^{(l)}\|_2 &\leq \|(\delta_{[\ell]})_j^{(l)}\|_2 + \sum_{i=1}^{l-1} \|M_l \cdots M_{i+1}(\delta_{[\ell]})_j^{(i)}\|_2 \\ &\leq \sum_{i=2}^{l} \|(\delta_{[\ell]})_j^{(i)}\|_2 + \|M_l \cdots M_2(\delta_{[\ell]})_j^{(1)}\|_2, \\ &\leq d_\ell(l-1) \left(\max_{1 \leq s \leq p_h, j \geq s} \|(A_\ell)_j^{(s)}\|_2 + \mathcal{O}(\epsilon_{\ell,l}^{\frac{1}{2}}) \right) \widetilde{\gamma}_m + \|M_l \cdots M_2(\delta_{[\ell]})_j^{(1)}\|_2, \\ &\leq d_h(j_{p_h} - p_{h-1} - t_h + 1)^{0.5} \alpha \max_{p_{h-1} < s \leq p_h} |(\delta R_{[\ell-1]})_{sj}|, \\ \|\Psi_{j,l}^{(i)}(\Delta_{l-i+1}^{(l-i)})\|_2 &\leq \alpha S_h^{R_{[\ell]}^d}(i+1)^{1/2} \|M_l M_{l-1} \cdots M_{l-i+1} \Delta_{l-i+1}^{(l-i)}\|_2 \\ &\leq \alpha S_h^{R_{[\ell]}^d}(i+1)^{1/2} \left(\sum_{s=2}^{l-i} \|(\delta_{[\ell]})_{l-i+1}^{(s)}\|_2 + \|M_l M_{l-1} \cdots M_2(\delta_{[\ell]})_{l-i+1}^{(1)}\|_2 \right) \\ &\sim \mathcal{O}(d_\ell \widetilde{\gamma}_m), \quad for \ \ 1 \leq i < l. \end{aligned} \tag{26}$$

Thus when $l = p_{h-1} + t_h - 1 \geq 0$, from (19) and (23)–(26), we derive that

$$\|(\xi_{[\ell]})_j^{(p_{h-1}+t_h)}\|_2 \leq d_h (j_{p_h} - p_{h-1} - t_h + 1)^{0.5} \alpha \max_{p_{h-1} < s \leq p_h} |(\delta R_{[\ell\,-\,1]})_{sj}|, \tag{27}$$

holds for $1 \leq h \leq \ell - 1,\ t_h = p_h - p_{h-1}$.

Step 3. Deduce the upper bound of $\|(\xi_{[\ell]})_j^{(l+1)}\|_2$, where

$$l = p_{\ell-1} + t_\ell - 1,\ \ t_\ell = 1 : p_\ell - p_{\ell-1} + 1,\ \ j \geq p_{\ell-1} + t_\ell.$$

We assume that

$$\max_{1 \leq s \leq p_{\ell-1}, h \geq s} |(\delta R_{[\ell\,-\,1]})_{sh}| / \min_{1 \leq s \leq p_{\ell-1}} (R_{[\ell\,-\,1]})_{ss} \leq \widetilde{\gamma}_m N_{[\ell\,-\,1]}. \tag{28}$$

By (17), (21) and (24), one can derive for $j \geq p_{\ell-1} + t_\ell$ that

$$\begin{aligned}
&\|M_{p_{\ell-1}} \cdots M_2 (\delta_{[\ell]})_j^{(1)}\|_2 \\
&\leq \|M_{p_{\ell-1}} \cdots M_1 (\xi_{[\ell]})_j^{(1)}\|_2 + \alpha \|M_1 (\xi_{[\ell]})_1^{(1)}\|_2 + \|(\overline{\delta}_{[\ell]})_j^{(1)})\|_2 \\
&\leq \alpha d_\ell \sum_{s=1}^{p_{\ell-1}} \frac{|(\delta R_{[\ell\,-\,1]})_{sj}|}{|(R_{[\ell\,-\,1]})_{ss}|} \|(A_\ell)_s^{(s)}\|_2 + \alpha d_\ell \frac{|(\delta R_{[\ell\,-\,1]})_{11}|}{|(R_{[\ell\,-\,1]})_{11}|} \|(A_\ell)_1^{(1)}\|_2 \\
&\qquad + d_\ell \widetilde{\gamma}_m \max\nolimits_{j \geq 1} \|(A_\ell)_j^{(1)}\|_2 + \mathcal{O}(d_\ell \epsilon_{\ell,1}^{\frac{1}{2}} \widetilde{\gamma}_m) \\
&\leq d_\ell (p_{\ell-1} + 2) \widetilde{\gamma}_m N_{[\ell\,-\,1]} \zeta_{[\ell\,-\,1,\,\ell]}.
\end{aligned}$$

Combining this with the estimates in (23) and (24), we have

$$\begin{aligned}
&\|\Delta_j^{(l)}\|_2 \leq \|(\delta_{[\ell]})_j^{(\ell)}\|_2 + \sum_{i=1}^{l-1} \|M_l \cdots M_{i+1} (\delta_{[\ell]})_j^{(i)}\|_2 \\
&\quad \leq \left(\sum_{i=2}^{p_{\ell-1}} + \sum_{i=p_{\ell-1}+1}^{l} \right) \|(\delta_{[\ell]})_j^{(i)}\|_2 + \|M_{p_{\ell-1}} \cdots M_2 (\delta_{[\ell]})_j^{(1)}\|_2 \\
&\quad \leq d_\ell p_{\ell-1} \widetilde{\gamma}_m N_{[\ell\,-\,1]} \zeta_{[\ell\,-\,1,\,\ell]} + d_\ell (t_\ell - 1) \widetilde{\gamma}_m (R_{[\ell]})_{p_{\ell-1}+1, p_{\ell-1}+1}, \\
&\|\Psi_{j,l}^{(i)}(\Delta_{l-i+1}^{(l-i)})\|_2 \leq \alpha S_\ell^{R_{[\ell]}^d} (i+1)^{\frac{1}{2}} \|M_l M_{l-1} \cdots M_{l-i+1} \Delta_{l-i+1}^{(l-i)}\|_2 \\
&\quad \leq \alpha S_\ell^{R_{[\ell]}^d} (i+1)^{\frac{1}{2}} \left(\sum_{s=2}^{l-i} \|(\delta_{[\ell]})_j^{(s)}\|_2 + \|M_{p_{\ell-1}} \cdots M_2 (\delta_{[\ell]})_{l-i+1}^{(1)}\|_2 \right) \\
&\quad \leq d_\ell S_\ell^{R_{[\ell]}^d} (i+1)^{\frac{1}{2}} \widetilde{\gamma}_m \Big(p_{\ell-1} N_{[\ell\,-\,1]} \zeta_{[\ell\,-\,1,\,\ell]} + \max\{t_\ell - i - 1, 0\} (R_{[\ell]})_{p_{\ell-1}+1, p_{\ell-1}+1} \Big).
\end{aligned} \tag{29}$$

Thus when $l = p_{\ell-1} + t_\ell - 1$, we derive from (23), (24) and (29) that

$$\begin{aligned}
&\|(\xi_{[\ell]})_j^{(p_{\ell-1}+t_\ell)}\|_2 \\
&\leq d_\ell S_\ell^{R_{[\ell]}^d} \widetilde{\gamma}_m \sum_{i=0}^{l-1} (i+1)^{\frac{1}{2}} \Big(p_{\ell-1} N_{[\ell\,-\,1]} \zeta_{[\ell\,-\,1,\,\ell]} + \max\{t_\ell - i - 1, 0\} (R_{[\ell]})_{p_{\ell-1}+1, p_{\ell-1}+1} \Big) \\
&\leq d_\ell S_\ell^{R_{[\ell]}^d} \widetilde{\gamma}_m \Big(p_{\ell-1} (p_{\ell-1} + t_\ell)^{1.5} N_{[\ell\,-\,1]} \zeta_{[\ell\,-\,1,\,\ell]} + t_\ell^{2.5} (R_{[\ell]})_{p_{\ell-1}+1, p_{\ell-1}+1} \Big).
\end{aligned} \tag{30}$$

Step 4. In this stage, we prove the following inequality inductively:

$$\|(\xi_{[\ell]})_j^{(p_{h-1}+t_h)}\|_2 \leq d_h \widetilde{\phi}_{t_h,\ell}^{(h)} \widetilde{\gamma}_m \max_{1 \leq i \leq p_h, j \geq i} (R_{[\ell]})_{ij}, \tag{31}$$

holds for $\ell = 2 : k, h = 1 : \ell, t_h = 1 : \delta_{h,\ell} + p_h - p_{h-1}$.

When $\ell=2$, using the forward roundoff error estimates in [20],

$$|(\delta R_{[1]})_{sj}| \le \phi_s^{(1)}\widetilde{\gamma}_m (R_{[1]})_{11}, \quad s=1:p_1, j=l:n,$$

and (27), (28), (30), one can verify that (31) follows for $\ell=2$.

Assume (31) holds for $\ell=s$. Then from (15), (16) and the standard roundoff error estimates, we have

$$\begin{aligned}
|(\delta R^d_{[s]})_{lj}| &= |fl\left(\widehat{q}_l^T(\overline{\Gamma}_{[s]})_j^{(l)}\right) - q_l^T(\Gamma_{[s]})_j^{(l)}| \\
&\le \|(\xi_{[s]})_j^{(l)}\|_2 + \alpha\|(\xi_{[s]})_l^{(l)}\|_2 + \widetilde{\gamma}_m \frac{|(\overline{\Gamma}_{[s]})_l^{(l)}|^T|(\overline{\Gamma}_{[s]})_j^{(l)}|}{\|(\overline{\Gamma}_{[s]})_l^{(l}\|_2} \\
&\le \|(\xi_{[s]})_j^{(l)}\|_2 + \alpha\|(\xi_{[s]})_l^{(l)}\|_2 + \begin{cases} d_l\widetilde{\gamma}_m|(R_{[s-1]})_{lj}|, & p_{h-1}<l\le p_h\le p_{s-1}, \\ d_s\widetilde{\gamma}_m\|(\overline{\Gamma}_{[s]})_j^{(l)}\|_2, & p_{s-1}<l\le p_s, \end{cases} \\
&\le \|(\xi_{[s]})_j^{(l)}\|_2 + \alpha\|(\xi_{[s]})_l^{(l)}\|_2 + \begin{cases} d_l\widetilde{\gamma}_m|(R_{[s]})_{lj}|, & p_{h-1}<l\le p_h\le p_{s-1}, \\ d_s\widetilde{\gamma}_m(R_{[s]})_{p_{s-1}+1,p_{s-1}+1}, & p_{s-1}<l\le p_s, \end{cases}
\end{aligned}$$

where $\alpha\sim 1$. Thus from the induction hypothesis, we obtain

$$|(\delta R_{[s]})_{p_{h-1}+t_h,j}| \le \widetilde{\phi}_{t_h,s}^{(h)}\widetilde{\gamma}_m \max_{1\le i\le p_h, j\ge i}|(R_{[s]})_{ij}|,\ h=1:s. \tag{32}$$

Thus for $\ell=s+1$, from (27), (28), (30) and (32) we derive for $h=1:s$ that

$$\begin{aligned}
\|(\xi_{[s+1]})_j^{(p_{h-1}+t_h)}\|_2 &\le d_h(j_{p_h}-p_{h-1}-t_h+1)^{0.5}\widetilde{\gamma}_m \max_{t_h}\widetilde{\phi}_{t_h,s}^{(h)} \max_{1\le i\le p_h, j\ge i}|(R_{[s]})_{ij}| \\
&\le d_h\widetilde{\gamma}_m\widetilde{\phi}_{t_h,s+1}^{(h)} \max_{1\le i\le p_h, j\ge i}|(R_{[s]})_{ij}|, \\
\|(\xi_{[s+1]})_j^{(p_s+t_{s+1}+1)}\|_2 &\le d_{s+1}(p_s+t_{s+1})^{2.5} S_{s+1}^{R^d_{[s+1]}} \frac{\zeta_{[s,s+1]}}{\min_{1\le l\le p_s}(R_{[d]})_{ll}} \times \\
&\quad \times\widetilde{\gamma}_m\widetilde{\phi}_{p_s-p_{s-1},s}^{(s)} \max_{1\le i\le p_s, j\ge i}|(R_{[s]})_{ij}| \\
&\le d_{s+1}\widetilde{\gamma}_m\widetilde{\phi}_{t_{s+1},s+1}^{(s+1)} \max_{1\le i\le p_{s+1}, j\ge i}|(R_{[s]})_{ij}|,
\end{aligned}$$

and therefore by induction procedure, (31) holds for $h=1:\ell, t_h=1:\delta_{h,\ell}+p_h-p_{h-1}$.

To bound $|(\overline{z}_{[\ell]})_{p_{h-1}+t_h,j}-(z_{[\ell]})_{p_{h-1}+t_h,j}|, \|(\overline{g}_{[\ell]})^{(p_{h-1}+t_h+1)}-(g_{[\ell]})^{(p_{h-1}+t_h+1)}\|_2$, we can regard $\overline{g}_{[\ell]}^{(1)}$ as the $(n+1)$-st column of $\overline{\Gamma}_{[\ell]}^{(1)}$. We can not allow the $(n+1)$-st column to participate in the column interchanges, so we should pre-multiply $\overline{g}_{[\ell]}^{(1)}$ by ζ_c^{-1}, and then apply the error estimates of

$$|(\overline{R}_{[\ell]})_{p_{h-1}+t_h,j}-(R_{[\ell]})_{p_{h-1}+t_h,j}|,\ \ \|(\overline{\Gamma}_{[\ell]})_j^{(p_{h-1}+t_h)}-(\Gamma_{[\ell]})_j^{(p_{h-1}+t_h)}\|_2$$

to evaluate

$$|(\overline{z}_{[\ell]})_{p_{h-1}+t_h,j}-(z_{[\ell]})_{p_{h-1}+t_h,j}|,\ \ \|(\overline{g}_{[\ell]})^{(p_{h-1}+t_h)}-(g_{[\ell]})^{(p_{h-1}+t_h)}\|_2.$$

This completes the proof of Theorem 4.1.

4.3. Backward roundoff error of the RBPMGS

Theorem 4.2. *Under the notations in* (10)–(13)*, consider the RBPMGS of* $[DA, Db]$*, and let* Π *be the permutation matrix taking account of all column interchanges during the RBPMGS.*

Then there exists $(nk+m)\times(nk+m)$ *orthogonal matrices* $\widehat{P}$ *such that*

$$\begin{pmatrix} \Delta E_k^d\Pi & \Delta h_k^d \\ \Delta E_{k-1}^d\Pi & \Delta h_{k-1}^d \\ \vdots & \vdots \\ \Delta E_1^d\Pi & \Delta h_1^d \\ d_1A_1\Pi+\Delta A_1^d\Pi & d_1b_1+\Delta b_1^d \\ \vdots & \vdots \\ d_kA_k\Pi+\Delta A_k^d\Pi & d_kb_k+\Delta b_k^d \end{pmatrix} = \widehat{P}\begin{pmatrix} \overline{R}_{[k]}^d & \overline{z}_{[k]}^d \\ \overline{R}_{[k-1]}^{d(p_k+1)} & \overline{z}_{[k-1]}^{d(p_k+1)} \\ \vdots & \vdots \\ \overline{R}_{[1]}^{d(p_2+1)} & \overline{z}_{[1]}^{d(p_2+1)} \\ d_1\overline{A}_1^{(p_1+1)} & d_1\overline{b}_1^{(p_1+1)} \\ \vdots & \vdots \\ d_k\overline{A}_k^{(p_k+1)} & d_k\overline{b}_k^{(p_k+1)} \end{pmatrix}, \tag{33}$$

where $\widehat{P}=\widehat{P}^{(1)}\cdots\widehat{P}^{(k)},\widehat{P}^{(j)}=\widehat{P}_1^{(j)}\cdots\widehat{P}_{p_j}^{(j)}$, *where*

$$\widehat{P}_l^{(j)}=I-\widehat{v}_l^{(j)}\widehat{v}_l^{(j)^T},\qquad \widehat{v}_l^{(j)}=\begin{pmatrix} 0 \\ -e_l \\ \frac{(\overline{R}_{[j-1]}^d)_l^{(l)}}{(\overline{R}_{[j]}^d)_{ll}} \\ 0 \\ \frac{d_j(\overline{A}_j)_l^{(l)}}{(\overline{R}_{[j]}^d)_{ll}} \\ 0 \end{pmatrix}\begin{matrix} n(k-j) \\ n \\ n_j \\ n(j-1)-n_j+\sum_{s=1}^{j-1}m_s \\ m_j \\ \sum_{s=j+1}^{k}m_s \end{matrix}. \tag{34}$$

Here, $n_1=0$ *and* $n_j=n$ *for* $j\geq 2$, *and*

$$\begin{aligned} &|\Delta E_s^d\Pi|\leq\widetilde{\gamma}_m\mathcal{P}'_{s,k-1}\Omega_1^{(s)}ee^T\mathrm{diag}(1,2,\cdots,p_k,\cdots,p_k)^2,\ \ s=1:k-1,\\ &|\Delta A_s^d\Pi|\leq\widetilde{\gamma}_m\mathcal{P}''_{s,k-1}\Omega_{s2}^{(s)}ee^T\mathrm{diag}(1,2,\cdots,p_k,\cdots,p_k)^2,\ \ s=1:k-1,\\ &|\Delta E_k^d\Pi|\leq\widetilde{\gamma}_m\Omega_1^{(k)}ee^T\mathrm{diag}(1,2,\cdots,p_k,\cdots,p_k),\\ &|\Delta A_k^d\Pi|\leq\widetilde{\gamma}_m\Omega_{k2}^{(k)}ee^T\mathrm{diag}(1,2,\cdots,p_k,\cdots,p_k)^2,\\ &|\Delta h_s^d|\leq\widetilde{\gamma}_m\mathcal{P}'_{sk}\zeta_r\Omega_1^{(s)}e,\qquad |\Delta b_s^d|\leq\widetilde{\gamma}_m\mathcal{P}''_{sk}\zeta_r\Omega_{s2}^{(s)}e,\ \ s=1:k, \end{aligned} \tag{35}$$

where $e=[1,\cdots,1]^T,\zeta_r$ *is defined in* (13),

$$\begin{aligned} &\mathcal{P}'_{st}=p_s\prod_{i=s+1}^{t}p_i^2,\quad \mathcal{P}''_{st}=\prod_{i=s}^{t}p_i^2,\\ &\Omega_1^{(s)}=\mathrm{diag}((\overline{R}_{[s]}^d)_{11},\cdots,(\overline{R}_{[s]}^d)_{p_s,p_s},0_{n-p_s}),\ \ s=1:k,\\ &\Omega_{s2}^{(s)}=\mathrm{diag}(\alpha_{n_s+1}^{(s)},\cdots,\alpha_{n_s+m_s}^{(s)}),\ \ s=1:k. \end{aligned} \tag{36}$$

Proof. For simplicity we consider the RBPMGS of $(DA^{(1)},Db)$ without column pivoting, in which $A^{(1)}=A\Pi$.

Step 1. From the backward error estimates in ([20], Theorem 3.1), we derive the backward roundoff errors of p_1 times PMGS performed on $d_1A_1^{(1)}$ satisfy

$$\begin{pmatrix} 0_{n(k-1)} \\ \Delta\widetilde{E}_1^d \\ d_1A_1^{(1)}+\Delta\widetilde{A}_1^d \\ d_2A_2^{(1)} \\ \vdots \\ d_kA_k^{(1)} \end{pmatrix}=\widehat{P}^{(1)}\begin{pmatrix} 0_{n(k-1)} \\ \overline{R}_{[1]}^d \\ d_1\overline{A}_1^{(p_1+1)} \\ d_2A_2^{(1)} \\ \vdots \\ d_kA_k^{(1)} \end{pmatrix}, \tag{37}$$

where

$$|\Delta \widetilde{E}_1^d| \le \widetilde{\gamma}_m \Omega_1^{(1)} ee^T \mathrm{diag}(1,2,\cdots,p_1,\cdots,p_1),$$
$$|\Delta \widetilde{A}_1^d| \le \widetilde{\gamma}_m \Omega_{12}^{(1)} ee^T \mathrm{diag}(1,2,\cdots,p_1,\cdots,p_1)^2. \tag{38}$$

Also, similar to the proof of Theorem 3.1 in [20], one can prove that the backward roundoff error estimates of p_1 times MMGS and $p_2 - p_1$ times MGS performed on $\begin{pmatrix} \overline{R}_{[1]}^d \\ d_2 A_2^{(1)} \end{pmatrix}$ also satisfy

$$\begin{pmatrix} 0_{n(k-2)} \\ \Delta \tilde{E}_2^d \\ \overline{R}_{[1]}^d + \Delta \overline{R}_{[1]}^d \\ d_1 \overline{A}_1^{(p_1+1)} \\ d_2 A_2^{(1)} + \Delta \widetilde{A}_2^d \\ \vdots \\ d_k A_k^{(1)} \end{pmatrix} = \widehat{P}^{(2)} \begin{pmatrix} 0_{n(k-2)} \\ \overline{R}_{[2]}^d \\ \overline{R}_{[1]}^{d^{(p_2+1)}} \\ d_1 \overline{A}_1^{(p_1+1)} \\ d_2 \overline{A}_2^{(p_2+1)} \\ \vdots \\ d_k A_k^{(1)} \end{pmatrix}, \tag{39}$$

where

$$|\Delta \widetilde{E}_2^d| \le \widetilde{\gamma}_m \Omega_1^{(2)} ee^T \mathrm{diag}(1,2,\cdots,p_2,\cdots,p_2),$$
$$\left| \begin{pmatrix} \Delta \overline{R}_{[1]}^d \\ \Delta \widetilde{A}_2^d \end{pmatrix} \right| \le \widetilde{\gamma}_m \Omega^{(2)} ee^T \mathrm{diag}(1,2,\cdots,p_2,\cdots,p_2)^2. \tag{40}$$

Here,

$$\Omega^{(2)} = \mathrm{diag}(\alpha_i^{(2)})_{i=1}^{n+m_2}.$$

Pre-multiplying (39) by $\widehat{P}^{(1)}$, and observing the structure of $\widehat{P}^{(1)}$ and (37), we derive

$$\begin{pmatrix} 0_{n(k-2)} \\ \Delta \widetilde{E}_2^d \\ \Delta \widetilde{E}_1^d \\ d_1 A_1^{(1)} + \Delta \widetilde{A}_1^d \\ d_2 A_2^{(1)} + \Delta \widetilde{A}_2^d \\ \vdots \\ d_k A_k^{(1)} \end{pmatrix} + \widehat{P}^{(1)} \begin{pmatrix} 0_n \\ \vdots \\ 0_n \\ \Delta \overline{R}_{[1]}^d \\ 0_{m_1} \\ \vdots \\ 0_{m_k} \end{pmatrix} = \widehat{P}^{(1)} \widehat{P}^{(2)} \begin{pmatrix} 0_{n(k-2)} \\ \overline{R}_{[2]}^d \\ \overline{R}_{[1]}^{d^{(p_2+1)}} \\ d_1 \overline{A}_1^{(p_1+1)} \\ d_2 \overline{A}_2^{(p_2+1)} \\ \vdots \\ d_k A_k^{(1)} \end{pmatrix}.$$

Continue to considering the backward roundoff error estimates of p_{j-1} times MMGS and $p_j - p_{j-1}$ times MGS performed on $\begin{pmatrix} \overline{R}_{[j-1]}^d \\ d_j A_j^{(1)} \end{pmatrix}$ for $j = 3, \cdots, t$. Then one can inductively prove

$$\begin{pmatrix} 0_{n(k-t)} \\ \Delta \widetilde{E}_t^d \\ \vdots \\ \Delta \widetilde{E}_1^d \\ d_1 A_1^{(1)} + \Delta \widetilde{A}_1^d \\ \vdots \\ d_t A_t^{(1)} + \Delta \widetilde{A}_t^d \\ \vdots \\ d_k A_k^{(1)} \end{pmatrix} + \sum_{s=1}^{t-1} \widehat{P}^{(1)} \cdots \widehat{P}^{(s)} \begin{pmatrix} 0_{n(k-s)} \\ \Delta \overline{R}_{[s]}^d \\ 0_n \\ \vdots \\ 0_n \\ 0_{m_1} \\ \vdots \\ 0_{m_k} \end{pmatrix} = \widehat{P}^{(1)} \cdots \widehat{P}^{(t)} \begin{pmatrix} 0_{n(k-t)} \\ \overline{R}_{[t]}^d \\ \overline{R}_{[t-1]}^{d^{(p_t+1)}} \\ \vdots \\ d_1 \overline{A}_1^{(p_1+1)} \\ \vdots \\ d_t \overline{A}_t^{(p_t+1)} \\ \vdots \\ d_k A_k^{(1)} \end{pmatrix}, \tag{41}$$

holds for $t = 2 : k$, where

$$
\begin{array}{l}
|\Delta \widetilde{E}_s^d| \le \widetilde{\gamma}_m \Omega_1^{(s)} ee^T \mathrm{diag}(1, 2, \cdots, p_s, \cdots, p_s), \ \ s = 1 : t, \\
|\Delta \widetilde{A}_1^d| \le \widetilde{\gamma}_m \Omega_{12}^{(1)} ee^T \mathrm{diag}(1, 2, \cdots, p_1, \cdots, p_1), \\
|\begin{pmatrix} \Delta \overline{R}_{[s-1]}^d \\ \Delta \widetilde{A}_s^d \end{pmatrix}| \le \widetilde{\gamma}_m \Omega^{(s)} ee^T \mathrm{diag}(1, 2, \cdots, p_s, \cdots, p_s)^2, \\
\Omega^{(s)} = \mathrm{diag}(\alpha_i^{(s)})_{i=1}^{n+m_s}, \ \ s \ge 2.
\end{array}
\tag{42}
$$

Here, the j-st $(p_{s-1} + 1 \le j \le n)$ diagonal entries of $\Omega^{(s)} (s \ge 2)$ are all zero.
Step 2. Evaluate the upper bound of the second term in the left side of (41). Denote

$$
\overline{H}^{(s+1)} \equiv (0, \Delta \overline{R}_{[s]}^{d^T}, 0)^T, \quad \overline{H}^{(\ell)} \equiv \widehat{P}_\ell \overline{H}^{(\ell+1)} \equiv \widehat{P}^{(\ell)} \cdots \widehat{P}^{(s)} \overline{H}^{(s+1)},
$$

for $\ell = s, s-1, \cdots, 1$. Thus from $\widehat{P}_j^{(s)} = I - \widehat{v}_j^{(s)} \widehat{v}_j^{(s)^T}$ we derive

$$
\begin{aligned}
\overline{h}_j^{(s)} &= \widehat{P}^{(s)} \overline{h}_j^{(s+1)} = \widehat{P}_1^{(s)} \cdots \widehat{P}_{p_s}^{(s)} \overline{h}_j^{(s+1)} \\
&= \widehat{P}_1^{(s)} \cdots \widehat{P}_{p_s-1}^{(s)} \overline{h}_j^{(s+1)} - (\widehat{v}_{p_s}^{(s)^T} \overline{h}_j^{(s+1)}) \widehat{P}_1^{(s)} \cdots \widehat{P}_{p_s-1}^{(s)} \widehat{v}_{p_s}^{(s)} \\
&= \cdots \\
&= h_j^{(s+1)} - \sum_{i=1}^{p_s} (\widehat{v}_i^{(s)^T} \overline{h}_j^{(s+1)}) \widehat{P}_1^{(s)} \cdots \widehat{P}_{i-1}^{(s)} \widehat{v}_i^{(s)},
\end{aligned}
\tag{43}
$$

where

$$
\begin{array}{l}
|\widehat{P}_1^{(s)} \cdots \widehat{P}_{i-1}^{(s)} \widehat{v}_i^{(s)}| = |(I - \widehat{v}_1^{(s)} \widehat{v}_1^{(s)^T}) \widehat{P}_2^{(s)} \cdots \widehat{P}_{i-1}^{(s)} \widehat{v}_i^{(s)}| \\
\le |\widehat{P}_2^{(s)} \cdots \widehat{P}_{i-1}^{(s)} \widehat{v}_i^{(s)}| + |\widehat{v}_1^{(s)}| |\widehat{v}_1^{(s)^T} \widehat{P}_2^{(s)} \cdots \widehat{P}_{i-1}^{(s)} \widehat{v}_i^{(s)}| \\
\le \cdots \\
\le |\widehat{v}_i^{(s)}| + \sum_{l=1}^{i-1} (|\widehat{v}_l^{(s)^T} \widehat{P}_{l+1}^{(s)} \cdots \widehat{P}_{i-1}^{(s)} \widehat{v}_i^{(s)}|) |\widehat{v}_l^{(s)}| \\
\le |\widehat{v}_i^{(s)}| + 2 \sum_{l=1}^{i-1} |\widehat{v}_l^{(s)}| \le 2 \sum_{l=1}^{i} |\widehat{v}_l^{(s)}| \qquad (\text{because } \|\widehat{v}_i^{(s)}\|_2 = \sqrt{2}).
\end{array}
\tag{44}
$$

From the structure of $\widehat{v}_i^{(s)}$ in (34) and the roundoff error estimates in (42), we obtain

$$
|\widehat{v}_i^{(s)^T} \overline{h}_j^{(s+1)}| = |(\Delta \overline{R}_{[s]}^d)_{ij}| \le \min\{j^2, p_{s+1}^2\} \widetilde{\gamma}_m \alpha_i^{(s+1)},
\tag{45}
$$

where $\alpha_i^{(s+1)}$ for $1 \le i \le p_s$ is bounded by (15) as

$$
\begin{array}{l}
\alpha_i^{(s+1)} = \max\limits_{\substack{1 \le t \le p_{s+1} \\ j \ge t}} |(\overline{\Gamma}_{[s+1]})_{ij}^{(t)}| = \beta (\overline{R}_{[s]}^d)_{ii} = \beta \alpha_i^{(s)}, \ \ \beta \sim 1, \\
|\widehat{v}_i^{(s)^T} \overline{h}_j^{(s+1)}| = |(\Delta \overline{R}_{[s]}^d)_{ij}| \le \min\{j^2, p_{s+1}^2\} \widetilde{\gamma}_m (\overline{R}_{[s]}^d)_{ii}.
\end{array}
\tag{46}
$$

Thus from (43)–(46), we derive

$$
\begin{aligned}
|\overline{h}_j^{(s)}| &\le |\overline{h}_j^{(s+1)}| + 2 \sum_{i=1}^{p_s} |\widehat{v}_i^{(s)^T} \overline{h}_j^{(s+1)}| \sum_{l=1}^{i} |\widehat{v}_l^{(s)}| \\
&\le \min\{j^2, p_{s+1}^2\} \widetilde{\gamma}_m \left(\begin{pmatrix} 0_{n(k-s)} \\ \Omega_1^{(s)} e \\ 0_{m+n(s-1)} \end{pmatrix} + \sum_{i=1}^{p_s} (\overline{R}_{[s]}^d)_{ii} \sum_{l=1}^{i} |\widehat{v}_l^{(s)}| \right),
\end{aligned}
\tag{47}
$$

where

$$|\widehat{v}_l^{(1)}| \le [\bar{0}_{[1]}, e_l, \frac{\alpha_1^{(1)}}{(\overline{R}_{[1]}^d)_{ll}}, \cdots, \frac{\alpha_{m_1}^{(1)}}{(\overline{R}_{[1]}^d)_{ll}}, \tilde{0}_{[1]}]^T,$$

$$|\widehat{v}_l^{(s)}| \le [\bar{0}_{[s]}, e_l, \frac{\alpha_1^{(s)}}{(\overline{R}_{[s]}^d)_{ll}}, \cdots, \frac{\alpha_{p_{s-1}}^{(s)}}{(\overline{R}_{[s]}^d)_{ll}}, 0_{n-p_{s-1}}, \hat{0}_{[s]}, \frac{\alpha_{n+1}^{(s)}}{(\overline{R}_{[s]}^d)_{ll}}, \cdots, \frac{\alpha_{n+m_s}^{(s)}}{(\overline{R}_{[s]}^d)_{ll}}, \tilde{0}_{[s]}]^T, \ s \ge 2.$$

Here, $\bar{0}_{[s]}, \hat{0}_{[s]}, \tilde{0}_{[s]}$ denote zero vectors of order $n(k-s), n(s-2) + \sum_{j=1}^{s-1} m_j$ and $\sum_{j=s+1}^{k} m_j$, respectively.

Note $(\overline{R}_{[s]}^d)_{ll} \ge \beta(\overline{R}_{[s]}^d)_{ii}$ for $l \le i$. Then substitute (42) and (46) into (47) to obtain

$$\begin{aligned} |\overline{h}_j^{(s)}| &\le \min\{j^2, p_{s+1}^2\}\widetilde{\gamma}_m \Big\{ \begin{pmatrix} \bar{0}_{[s]} \\ \Omega_1^{(s)} e \\ 0_n \\ \hat{0}_{[s]} \\ 0_n \\ \tilde{0}_{[s]} \end{pmatrix} + \sum_{i=1}^{p_s} \sum_{l=1}^{i} \begin{pmatrix} \bar{0}_{[s]} \\ (\overline{R}_{[s]}^d)_{ii} e_l \\ \Omega_{s1}^{(s)} e \\ \hat{0}_{[s]} \\ \Omega_{s2}^{(s)} e \\ \tilde{0}_{[s]} \end{pmatrix} \Big\} \\ &\le \min\{j^2, p_{s+1}^2\}\widetilde{\gamma}_m \mathrm{diag}(\bar{0}_{[s]}, p_s\Omega_1^{(s)}, p_s^2\Omega_1^{(s-1)}, \hat{0}_{[s]}, p_s^2\Omega_{s2}^{(s)}, \tilde{0}_{[s]})e, \end{aligned}$$

where

$$\Omega_{s1}^{(s)} = \mathrm{diag}(\alpha_i^{(s)})_{i=1}^{n_s}, \Omega_{s2}^{(s)}$$

is defined by (36).

Step 3. Note that

$$\overline{H}^{(\ell-1)} = \widehat{P}^{(\ell-1)}\overline{H}^{(\ell)}.$$

Thus using the techniques in deducing (43)–(47), we can derive

$$|\overline{h}_j^{(\ell-1)}| \le |\overline{h}_j^{(\ell)}| + 2\sum_{i=1}^{p_{\ell-1}} (|\widehat{v}_i^{(\ell-1)}|^T |\overline{h}_j^{(\ell)}|) \sum_{l=1}^{i} |\widehat{v}_l^{(\ell-1)}| \tag{48}$$

and prove inductively that

$$\overline{h}_j^{(\ell)} = \widehat{P}^{(\ell)}\overline{h}_j^{(\ell+1)} = \widehat{P}_\ell \cdots \widehat{P}_s \overline{h}_j^{(s+1)}$$

for $\ell = s, \cdots, 1$ satisfy

$$\begin{aligned} |\overline{h}_j^{(\ell)}| \le \min\{j^2, p_{s+1}^2\}\widetilde{\gamma}_m \mathrm{diag}(&\bar{0}_{[s]}, \mathcal{P}'_{ss}\Omega_1^{(s)}, \mathcal{P}'_{s-1,s}\Omega_1^{(s-1)}, \cdots, \mathcal{P}'_{\ell s}\Omega_1^{(\ell)}, \\ &\mathcal{P}''_{\ell s}\Omega_1^{(\ell-1)}, \hat{0}_{[\ell]}, \mathcal{P}''_{\ell s}\Omega_{\ell 2}^{(\ell)}, \cdots, \mathcal{P}''_{s-1,s}\Omega_{s-1,2}^{(s-1)}, \mathcal{P}''_{ss}\Omega_{s2}^{(s)}, \tilde{0}_{[s]})e. \end{aligned}$$

Therefore,

$$\begin{aligned} |\overline{h}_j^{(1)}| \le \min\{j^2, p_{s+1}^2\}\widetilde{\gamma}_m \mathrm{diag}(&0_{[s]}, \mathcal{P}'_{ss}\Omega_1^{(s)}, \mathcal{P}'_{s-1,s}\Omega_1^{(s-1)}, \cdots, \mathcal{P}'_{1s}\Omega_1^{(1)}, \\ &\mathcal{P}''_{1s}\Omega_{12}^{(1)}, \mathcal{P}''_{2s}\Omega_{22}^{(2)}, \cdots, \mathcal{P}''_{ss}\Omega_{s2}^{(s)}, \tilde{0}_{[s]})e. \end{aligned} \tag{49}$$

Step 4. Take $t = k$ in (41). Then from the estimates in (49), we derive

$$\left|\sum_{s=1}^{k-1} \widehat{P}^{(1)} \cdots \widehat{P}^{(s)} \overline{h}_j^{(s+1)}\right| \le \sum_{s=1}^{k-1} |\overline{h}_j^{(1)}|$$
$$\le \min\{j^2, p_k^2\}\widetilde{\gamma}_m \mathrm{diag}(\bar{0}_{[k-1]}, \mathcal{P}'_{k-1,k-1}\Omega_1^{(k-1)}, \mathcal{P}'_{k-2,k-1}\Omega_1^{(k-1)}, \cdots,$$
$$\mathcal{P}'_{1,k-1}\Omega_1^{(1)}, \mathcal{P}''_{1,k-1}\Omega_{12}^{(1)}, \mathcal{P}''_{2,k-1}\Omega_{22}^{(2)}, \cdots, \mathcal{P}''_{k-1,k-1}\Omega_{k-1,2}^{(k-1)}, \tilde{0}_{[k-1]}).$$

Combining this with (41)–(42), and taking into account the permutation Π, we then prove the upper bounds of $\Delta E_i^d \Pi, \Delta A_i^d \Pi$ in (35).

To bound $|\Delta h_i^d|, |\Delta b_i^d|$ in (35), we may regard b as the $(n+1)$-st column of $A^{(1)}$. We can not allow the $(n+1)$-st column to participate in the column interchanges and improve the value of $\alpha_i^{(s)}$ during the algorithm, thus we should pre-multiply b by ζ_r^{-1} and then apply the error estimates of $\Delta E_i^d \Pi, \Delta A_i^d \Pi$ to evaluate $|\Delta h_i^d|, |\Delta b_i^d|$.

Remark 4.3. From Theorems 4.1 and 4.2, we see that our upper bounds on forward rounding errors of the RBPMGS algorithm degrade as k increases. Thus, a tacit assumption is that the number of row blocks k is not too large.

Remark 4.4. We derive from Theorem 4.1 and Theorem 3.1 (see [20]) that

$$\|(\overline{\Gamma}_{[1]})_j^{(p_1+1)}\|_2 \le d_1 \phi_{p_1}^{(1)} \widetilde{\gamma}_{m_1} (R_{[1]})_{11}, \quad j \ge p_1,$$
$$\|(\overline{\Gamma}_{[\ell]})_j^{(p_\ell+1)}\|_2 \le d_\ell \widetilde{\phi}_{p_\ell - p_{\ell-1},\ell}^{(\ell)} \widetilde{\gamma}_m \max_{1\le i\le p_\ell, j\ge i} |(R_{[l]})_{ij}|, \quad j = p_\ell + 1 : n,$$

for $\ell = 2 : k$. Thus if the number of row blocks k is not too large, and A is well-conditioned satisfying

$$\widetilde{\gamma}_m \phi_{p_1}^{(1)} (R_{[1]})_{11} \ll (R_{[1]})_{p_1,p_1},$$
$$\widetilde{\gamma}_m \widetilde{\phi}_{p_\ell - p_{\ell-1},\ell}^{(\ell)} \max_{1\le i\le p_\ell, j\ge i} |(R_{[\ell]})_{ij}| \ll (R_{[\ell]})_{p_\ell,p_\ell}, \quad \ell = 2 : k,$$

then we can choose tolerances η_ℓ to determine the numerical rank of C_ℓ, for $\ell = 1, 2, \cdots, k$.

Remark 4.5. Note that $\alpha_{n_s+i}^{(s)} / \max_j |d_s (A_s)_{ij}|, s = 1 : k$ are generally of unit order, as mentioned in [20]. From (35) we see that, if A is well conditioned and the number of row blocks k is not too large, then the RBPMGS is row-wise stable.

5. Numerical Examples

In this section, we provide some examples to compare the ordinary PMGS and the RBPMGS (Algorithm 3.1) for solving the stiff WLS problem Eq. (1). All the computations are performed on Matlab software with unit roundoff $u = 2.22e\text{-}16$. Denote

- $\delta x_{WLS} = \overline{x}_{WLS} - x_{WLS}$,
- Method 1 (M1): PMGS;
- Method 2 (M2): RBPMGS (Algorithm 3.1);
- $\|\delta x_{\mathrm{M1}}\|$: The 2-norm of δx_{WLS} using Method 1; and
- $\|\delta x_{\mathrm{M2}}\|$: The 2-norm of δx_{WLS} using Method 2.

Let

$$\beta^{\mathrm{M1}} = \max_{j\geq p_k+1} \|\overline{A}_j^{d(p_k+1)}\|, \quad \beta_\ell^{\mathrm{M2}} = \max_{j\geq p_\ell+1} \|(\overline{\Gamma}_{[\ell]})_j^{(p_\ell+1)}\|, \quad \ell = 1:k,$$

where $\overline{A}_j^{d(p_k+1)}$ is numerically computed from $A^d \equiv DA$ via p_k times PMGS, and $(\overline{\Gamma}_{[\ell]})_j^{(p_\ell+1)}$ is numerically computed from $(\overline{\Gamma}_{[\ell]})_j^{(p_\ell+1)}$ via $p_{\ell-1}$ times MMGS and $p_\ell - p_{\ell-1}$ times PMGS.

Example 5.1.

$$A = \begin{pmatrix} -4 & 2 & -3 \\ 4 & 2 & 2 \\ 2 & 1 & 1 \\ 1 & -1 & 1 \end{pmatrix}, \quad b = \begin{pmatrix} -9 \\ 4 \\ 1 \\ 4 \end{pmatrix}, \quad D = \mathrm{diag}(d_1, d_1, d_2, d_3).$$

Therefore, $\mathrm{rank}(A) = 3, \mathrm{rank}(A(1:3,:)) = 2$, A is of full rank, $\beta^{\mathrm{M1}} = 0$, and

$$x_{WLS} = (-3, 0, 7)^T + \frac{1}{4 + d_3^2}(-4, 4, 8).$$

Setting $b = A_{n+1}$, and applying M1 and M2 respectively on DA (do not interchange $(n+1)$-st column), we obtain the following numerical results as in Table 5.1.

Example 5.2.

$$A = \begin{pmatrix} 1 & 2 & 4 & 2 \\ 1 & 3 & 2 & 5 \\ 1 & 1 & 6 & -1 \\ 6 & 8 & 0 & 4 \\ 4 & 3 & -6 & -3 \end{pmatrix}, \quad b = \begin{pmatrix} 11 \\ -6 \\ 28 \\ 15 \\ 22 \end{pmatrix}, \quad D = \mathrm{diag}(d_1 I_3, d_2, d_3).$$

So $\mathrm{rank}(A) = 3, \mathrm{rank}(A(1:3,:)) = 2$, and A is rank-deficient,

$$x_{WLS} = \frac{1}{4500} z_1 + \frac{2d_3^2}{125(6(d_2^2 + d_3^2) + 11 d_2^2 d_3^2)} z_2,$$

where

$$z_1 = \begin{pmatrix} 12936 \\ 8017 \\ 14414 \\ -18563 \end{pmatrix}, \quad z_2 = \begin{pmatrix} 12(43d_2^2 + 35) \\ 152d_2^2 + 365 \\ -2(208d_2^2 + 85) \\ -1078d_2^2 - 235 \end{pmatrix}.$$

Setting $b = A_{n+1}$, and applying M1 and M2 respectively on DA (do not interchange $(n+1)$-st column), we obtain the following numerical results as in Table 5.2.

Example 5.3.

$$A = \begin{pmatrix} 1 & 2 & 4 & 2 & 6 \\ 1 & 3 & 2 & 5 & -5 \\ 1 & 1 & 6 & -1 & 17 \\ 1 & 1 & 1 & 1 & 1 \\ 1 & -1 & 0 & -3 & 7 \\ 9 & -5 & 7 & -6 & 1 \end{pmatrix}, \quad b = \begin{pmatrix} 23 \\ -16 \\ 62 \\ 2 \\ 41 \\ 51 \end{pmatrix}, \quad D = \mathrm{diag}(d_1 I_3, d_2, d_3, d_4).$$

Table 5.1. $d_1 = d_2 = 1 \geq d_3$.

d_3	1	e-2	e-4	e-6	e-8	e-12
$\|\delta x_{M1}\|_2$	1.99e-15	4.21e-15	2.22e-16	1.04e-14	9.98e-13	9.87e-5
$\|\delta x_{M2}\|_2$	1.99e-15	4.31e-15	4.31e-15	2.98e-15	2.04e-15	2.04e-15
β_1^{M2}	0	3.82e-16	3.82e-16	3.82e-16	3.82e-16	3.82e-16

Table 5.2. $d_1 = 1 \geq d_2 \geq d_3$.

d_2	1	e-4	e-6	e-8	e-10	e-12
d_3	1	e-4	e-6	e-8	e-10	e-12
$\|\delta x_{M1}\|_2$	1.78e-15	2.04e-15	3.17e-15	1.83e-15	2.00e-12	2.00e-8
$\|\delta x_{M2}\|_2$	1.78e-15	2.04e-15	2.04e-15	3.26e-15	2.74e-15	2.84e-15
β^{M1}	4.68e-16	1.71e-16	1.71e-16	3.88e-16	2.62e-16	2.62e-16
β_1^{M2}	4.68e-16	8.67e-16	8.67e-16	8.67e-16	8.67e-16	8.67e-16
β_2^{M2}	blank	2.42e-19	1.89e-21	2.73e-23	1.46e-25	1.14e-27

Table 5.3. $1 = d_1 = d_2 > d_3 \geq d_4$.

d_3	e-2	e-4	e-8	e-8	e-4	e-2
d_4	e-4	e-8	e-8	e-12	e-12	e-12
$\|\delta x_{M1}\|_2$	4.27e-13	4.21e-9	2.03e-15	5.10e-8	1.58e-1	9.51e+2
$\|\delta x_{M2}\|_2$	1.77e-15	3.35e-15	1.02e-15	2.36e-15	5.09e-16	1.98e-15
β^{M1}	2.33e-15	2.27e-15	9.55e-16	9.06e-16	1.94e-15	9.61e-16
β_1^{M2}	2.95e-15	2.95e-15	2.95e-15	2.95e-15	2.95e-15	2.95e-15
β_2^{M2}	6.98e-18	1.51e-19	7.74e-24	9.73e-24	1.51e-19	6.98e-18
β_3^{M2}	2.12e-22	6.24e-24	blank	1.20e-38	1.18e-38	2.21e-39

Table 5.4. $d_1 = 1 \geq d_2 \geq d_3 \geq d_4$.

d_2	1	e-4	e-4	1	1	1
d_3	1	e-4	e-4	1	e-4	1
d_4	e-4	e-4	e-8	e-8	e-8	e-12
$\|\delta x_{M1}\|_2$	1.65e-9	3.88e-15	3.42e-10	6.96e-2	4.21e-9	2.61e+6
$\|\delta x_{M2}\|_2$	1.84e-15	3.08e-15	6.37e-15	4.00e-15	3.35e-15	3.23e-15
β^{M1}	2.63e-15	3.12e-16	7.16e-16	1.41e-15	2.26e-15	1.27e-15
β_1^{M2}	1.54e-15	1.26e-15	1.26e-15	1.54e-15	2.95e-15	1.54e-15
β_2^{M2}	5.65e-23	7.13e-20	6.78e-21	1.32e-23	1.51e-19	1.18e-38
β_3^{M2}	blank	blank	1.85e-23	blank	6.62e-24	blank

So $\text{rank}(A) = 4, \text{rank}(A(1:3,:)) = 2, \text{rank}(A(1:4,:)) = 3$, and

$$x_{WLS} = \frac{1}{30934} z_1 + \frac{d_3^2}{30934(6(d_2^2 + 4d_3^2) + 5d_2^2 d_3^2)} z_2,$$

where

$$z_1 = \begin{pmatrix} -29418 \\ -79792 \\ 157140 \\ -47074 \\ 61012 \end{pmatrix}, \quad z_2 = \begin{pmatrix} 643188d_2^2 + 8314992 \\ 237951d_2^2 + 4603284 \\ -919758d_2^2 - 7349832 \\ -257250d_2^2 + 370944 \\ 295869d_2^2 + 1855980 \end{pmatrix}.$$

Setting $b = A_{n+1}$, and applying M1 and M2 respectively on DA (do not interchange $(n+1)$-st column), we obtain the following numerical results as in Tables 5.3 and 5.4.

It is observed from the above examples that if $d_1/d_k \gg 1$, and the first row block A_1 of A is not of full row rank, then computational results exhibit numerical instability when using the PMGS (Method 1), while the RBPMGS algorithm (Algorithm 3.1) gives a numerical solution with high precision. The quantities β^{M1} are of order $\mathcal{O}(d_1 p_k^{2.5} S^R \widetilde{\gamma}_m)$ and β_j^{M2} are of order $\mathcal{O}(d_j p_{[j]} \kappa_{[j]} \Upsilon_{[j]} \widetilde{\gamma}_m)$, where R is the accurately computed upper trapezoidal R-factor via p_k times MGS of $DA^{(1)}$. The numerical results agree with the estimates in (18).

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