Least upper bound of truncation error of low-rank matrix approximation algorithm using QR decomposition with pivoting

Haruka Kawamura¹ · Reiji Suda¹

Received: 31 May 2020 / Revised: 24 January 2021 / Accepted: 1 February 2021 /

Published online: 24 February 2021

© The Author(s) 2021

Abstract

Low-rank approximation by QR decomposition with pivoting (pivoted QR) is known to be less accurate than singular value decomposition (SVD); however, the calculation amount is smaller than that of SVD. The least upper bound of the ratio of the truncation error, defined by $\|A - BC\|_2$, using pivoted QR to that using SVD is proved to be $\sqrt{\frac{4^k-1}{3}(n-k)+1}$ for $A \in \mathbb{R}^{m \times n}$ ($m \geq n$), approximated as a product of $B \in \mathbb{R}^{m \times k}$ and $C \in \mathbb{R}^{k \times n}$ in this study.

Keywords Error analysis · Pivoting · QR decomposition · Singular values

Mathematics Subject Classification 65F55 · 15A45

1 Introduction

1.1 Low-rank approximation

Low-rank matrix approximation involves approximating a matrix by a matrix whose rank is less than that of the original matrix. Let $A \in \mathbb{R}^{m \times n}$; then, a rank k approximation of A is given by

$$A \approx BC$$

where $B \in \mathbb{R}^{m \times k}$ and $C \in \mathbb{R}^{k \times n}$. Low-rank matrix approximation appears in many applications such as data mining [5] and machine learning [14]. It also plays an important role in tensor decompositions [12].

✉ Reiji Suda
reiji@is.s.u-tokyo.ac.jp

Haruka Kawamura
kawamulahaluka@gmail.com

¹ The University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo 113-8656, Japan

This paper discusses truncation errors of low-rank matrix approximation using QR decomposition with pivoting, or pivoted QR. In this study, rounding errors are not considered, and the norm used is basically 2-norm. $A \in \mathbb{R}^{m \times n}$ (without loss of generality, we assume that $m \geq n$) is approximated by a product of $B \in \mathbb{R}^{m \times k}$ and $C \in \mathbb{R}^{k \times n}$, and the truncation error is defined by $\|A - BC\|_2$.

It is well-known that for any matrix $A \in \mathbb{R}^{m \times n}$ ($m \geq n$), there are orthogonal matrices $U \in \mathbb{R}^{m \times m}$ and $V \in \mathbb{R}^{n \times n}$ and a diagonal matrix $\Sigma \in \mathbb{R}^{n \times n}$ with nonnegative diagonal elements that satisfy

$$A = U \begin{pmatrix} \Sigma \\ O \end{pmatrix} V^T.$$

This is a singular value decomposition (SVD) of A . We define $\sigma_i(A)$ for $i = 1, 2, \dots, n$, satisfying

$$\text{diag}(\sigma_1(A), \sigma_2(A), \dots, \sigma_n(A)) = \Sigma,$$

and assume that $\sigma_1(A) \geq \sigma_2(A) \geq \dots \geq \sigma_n(A) \geq 0$ without loss of generality. The σ_i values are singular values of A . A has rank k if and only if $\sigma_k(A) > 0 = \sigma_{k+1}(A)$. Let

$$\Sigma_k = \text{diag}(\sigma_1(A), \sigma_2(A), \dots, \sigma_k(A)).$$

Then,

$$\begin{aligned} \min_{\text{rank}(X) \leq k} \|A - X\|_2 &= \left\| A - U \begin{pmatrix} \Sigma_k & O \\ O & O \end{pmatrix} V^T \right\|_2 \\ &= \sigma_{k+1}(A) \end{aligned}$$

holds [8]. Therefore, this is an A 's rank- k approximation whose 2-norm of truncation error is the smallest. We define the truncation error of low-rank approximation by SVD as

$$\text{SVD}_k(A) = \sigma_{k+1}(A).$$

The amount of computation required to calculate SVD is $O(nm \min(n, m))$.

Pivoted QR was proposed by Golub in 1965 [7]. Because the amount of computation required to calculate the low-rank approximation by pivoted QR is $O(nmk)$, it is cheaper than SVD and hence useful in many applications such as solving rank-deficient least squares problems [2]. It consists of QR decomposition and pivoting. For any matrix A , there exist $Q \in \mathbb{R}^{m \times n}$ and an upper triangular matrix $R \in \mathbb{R}^{n \times n}$ that satisfy $A = QR$ and $Q^T Q = I_n$. This is a QR decomposition of A . We use pivoting to determine the permutation matrix Π_{grd} and apply the QR decomposition algorithm to $A\Pi_{\text{grd}}$. The subscript *grd* signifies the greedy method, as explained previously. Hereafter, we redefine QR as a QR decomposition of $A\Pi_{\text{grd}} = QR$. Let Q and R be partitioned as

$$Q = (Q_{1k} \ Q_{2k}), R = \begin{pmatrix} R_{1k} & R_{2k} \\ O & R_{3k} \end{pmatrix}$$

where $Q_{1k} \in \mathbb{R}^{m \times k}$ and $R_{1k} \in \mathbb{R}^{k \times k}$. Then, we can approximate A to $Q_{1k} (R_{1k} \ R_{2k}) \Pi_{grd}^T$ and

$$\|A - Q_{1k} (R_{1k} \ R_{2k}) \Pi_{grd}^T\|_2 = \|R_{3k}\|_2$$

holds. We define the truncation error of low-rank approximation by pivoted QR as

$$pivotQR_k(A) = \|R_{3k}\|_2.$$

In this study, the greedy method is used to make $\|R_{3k}\|_2$ small in pivoting. Pivoting is performed such that the elements in $R = (r_{ij})$ satisfy the following inequalities [1, p.103]

$$r_{ll}^2 \geq \sum_{i=l}^j r_{ij}^2 \quad (l = 1, 2, \dots, n-1, j = l+1, l+2, \dots, n). \quad (1)$$

Condition (1) is not used to analyze the error for $l = k+1, k+2, \dots, n-1$.

The greedy method of pivoting is not always optimal. QR decompositions of $A\Pi_{RR}$, where Π_{RR} is chosen such that R_{RR} has a small lower right block and where $Q_{RR}R_{RR}$ is a QR decomposition of $A\Pi_{RR}$, are called rank-revealing QR (RRQR). The following theorem was shown by Hong et al. in 1992 [9].

Theorem 1 *Let $m \geq n > k$, and $A \in \mathbb{R}^{m \times n}$. Then, there exists a permutation matrix $\Pi \in \mathbb{R}^{n \times n}$ such that the diagonal blocks of $R = \begin{pmatrix} R_1 & R_2 \\ O & R_3 \end{pmatrix}$, the upper triangular factor of the QR decomposition of $A\Pi$ with $R_1 \in \mathbb{R}^{k \times k}$, satisfy the following inequality:*

$$\|R_3\|_2 \leq \sqrt{k(n-k) + \min(k, n-k)} \sigma_{k+1}(A).$$

Finding the optimal permutation matrix is not practical from the viewpoint of computational complexity.

1.2 Truncation error of pivoted QR

Pivoted QR sometimes results in a large truncation error. A well-known example was shown by Kahan, whose work we do not reproduce here [10]. In 1968, Faddeev et al. [6] showed that

$$pivotQR_{n-1}(A) \leq \frac{\sqrt{4^n + 6n - 1}}{3} SVD_{n-1}(A).$$

Furthermore,

$$\text{pivotQR}_k(A) \leq \frac{n\sqrt{4^k + 6k - 1}}{3} \text{SVD}_k(A)$$

holds [3].

However, in a survey in 2017, it was stated that “very little is known in theory about its behaviour” [13, p. 2218] with regard to pivoted QR, thus there is still room for further research on pivoted QR.

Our previous work showed that the least upper bound of the ratio of the truncation error of pivoted QR to that of SVD is $\sqrt{\frac{4^{n-1}+2}{3}}$ in case an $m \times n$ ($m \geq n$) matrix is approximated to a matrix whose rank is $n - 1$, i.e., for $k = n - 1$ [11]. The tight upper bound for all k is proved in the rest of this paper.

We assume that all matrices and vectors in this paper are real numbers; however, we can easily extend the discussion in this paper to complex numbers, and the same results can be obtained.

2 Preliminaries

In this section, we define the notations and examine the basic properties to analyze the truncation errors. First, we introduce the concept *resi*.

Proposition 1 [1, p. 16] *For $A \in \mathbb{R}^{m \times n}$, there exists $X \in \mathbb{R}^{n \times m}$ that satisfies*

$$AXA = A, XAX = X, (AX)^T = AX, (XA)^T = XA$$

and X is uniquely determined by the four conditions.

Definition 1 For $A \in \mathbb{R}^{m \times n}$ ($m \geq n$), the generalized inverse of A is defined by $X \in \mathbb{R}^{n \times m}$ that satisfies the four conditions in Proposition 1 and is denoted by $A^\dagger$.

The following notation is closely related to the truncation error of pivoted QR.

Definition 2 Let $A \in \mathbb{R}^{m \times n}$ ($m \geq n$) and $B \in \mathbb{R}^{m \times l}$. We define $\text{resi}(A, B)$ as

$$\text{resi}(A, B) = B - AA^\dagger B.$$

We denote the inner product of two vectors $\mathbf{x}$ and $\mathbf{y}$ as $(\mathbf{x}, \mathbf{y})$.

Example 1 For $\mathbf{x} \in \mathbb{R}^n$ and $\mathbf{y} \in \mathbb{R}^n$, if $\mathbf{x} \neq \mathbf{0}$, then the following holds:

$$\text{resi}(\mathbf{x}, \mathbf{y}) = \mathbf{y} - \frac{(\mathbf{x}, \mathbf{y})}{\|\mathbf{x}\|^2} \mathbf{x}.$$

The following lemma will be used to identify *resi*.

Lemma 1 Let $A \in \mathbb{R}^{m \times n}$ ($m \geq n$) and $B \in \mathbb{R}^{m \times l}$. For $X \in \mathbb{R}^{n \times l}$,

$$A^TAX - A^TB = O \Leftrightarrow \text{resi}(A, B) = B - AX$$

holds.

Proof If $\text{resi}(A, B) = B - AX$ holds, then

$$\begin{aligned} A^TAX - A^TB &= -A^T\text{resi}(A, B) = (A^TAA^\dagger - A^T)B \\ &= (A^T(AA^\dagger)^T - A^T)B = ((AA^\dagger A)^T - A^T)B = O \end{aligned}$$

holds. If $A^TAX - A^TB = O$ holds, then

$$\begin{aligned} \text{resi}(A, B) - B + AX &= AX - AA^\dagger B = AA^\dagger AX - AA^\dagger B \\ &= (AA^\dagger)^TAX - (AA^\dagger)^TB = A^{\dagger T}(A^TAX - A^TB) = O \end{aligned}$$

holds. □

Lemma 2 [1, p. 5] Let $A \in \mathbb{R}^{m \times n}$ ($m \geq n$), $\mathbf{b} \in \mathbb{R}^m$, and $\mathbf{x} \in \mathbb{R}^n$. $\|\mathbf{b} - A\mathbf{x}\| \leq \|\mathbf{b} - A\mathbf{y}\|$ holds for any $\mathbf{y} \in \mathbb{R}^n$ if and only if $A^T(A\mathbf{x} - \mathbf{b}) = \mathbf{0}$ holds.

Using Lemmas 1 and 2, we can obtain the following lemma.

Lemma 3 Let $A \in \mathbb{R}^{m \times n}$ ($m \geq n$), $\mathbf{b} \in \mathbb{R}^m$, and $\mathbf{x} \in \mathbb{R}^n$. $\|\mathbf{b} - A\mathbf{x}\| \leq \|\mathbf{b} - A\mathbf{y}\|$ holds for any $\mathbf{y} \in \mathbb{R}^n$ if and only if $\text{resi}(A, \mathbf{b}) = \mathbf{b} - A\mathbf{x}$ holds.

Lemma 4 Let $m \geq n > k$, $A \in \mathbb{R}^{m \times n}$, and $B \in \mathbb{R}^{m \times l}$. Let A be partitioned as

$$A = \begin{pmatrix} A_{1k} & A_{2k} \end{pmatrix}$$

where $A_{1k} \in \mathbb{R}^{m \times k}$. Then,

$$\text{resi}(A, B) = \text{resi}(\text{resi}(A_{1k}, A_{2k}), \text{resi}(A_{1k}, B))$$

holds.

Proof From the definition of resi , we can see that

$$\text{resi}(A_{1k}, A_{2k}) = A_{2k} - A_{1k}X, \quad (2)$$

$$\text{resi}(A_{1k}, B) = B - A_{1k}Y \quad (3)$$

and

$$\text{resi}(\text{resi}(A_{1k}, A_{2k}), \text{resi}(A_{1k}, B)) = \text{resi}(A_{1k}, B) - \text{resi}(A_{1k}, A_{2k})Z \quad (4)$$

hold where $X = A_{1k}^\dagger A_{2k}$, $Y = A_{1k}^\dagger B$ and $Z = \text{resi}(A_{1k}, A_{2k})^\dagger \text{resi}(A_{1k}, B)$. Thus,

$$\text{resi}(\text{resi}(A_{1k}, A_{2k}), \text{resi}(A_{1k}, B)) = B - A_{1k}Y - A_{2k}Z + A_{1k}XZ \quad (5)$$

holds from (2), (3), and (4). Lemma 1 proves

$$A_{1k}^T A_{2k} = A_{1k}^T A_{1k} X, \quad (6)$$

from (2),

$$A_{1k}^T B = A_{1k}^T A_{1k} Y \quad (7)$$

from (3), and

$$\text{resi}(A_{1k}, A_{2k})^T (\text{resi}(A_{1k}, B) - \text{resi}(A_{1k}, A_{2k})Z) = O \quad (8)$$

from (4). We can see that

$$\begin{aligned} & A_{1k}^T \text{resi}(\text{resi}(A_{1k}, A_{2k}), \text{resi}(A_{1k}, B)) \\ &= A_{1k}^T (B - A_{1k}Y - A_{2k}Z + A_{1k}XZ) \\ &= O \end{aligned} \quad (9)$$

from (5), (6), and (7). We can see that

$$\begin{aligned} & A_{2k}^T \text{resi}(\text{resi}(A_{1k}, A_{2k}), \text{resi}(A_{1k}, B)) \\ &= (A_{2k} - A_{1k}X)^T \text{resi}(\text{resi}(A_{1k}, A_{2k}), \text{resi}(A_{1k}, B)) \\ &= \text{resi}(A_{1k}, A_{2k})^T (\text{resi}(A_{1k}, B) - \text{resi}(A_{1k}, A_{2k})Z) \\ &= O \end{aligned} \quad (10)$$

from (2), (4), (8), and (9). Then, (9) and (10) can be combined as

$$\begin{aligned} & \begin{pmatrix} A_{1k}^T \\ A_{2k}^T \end{pmatrix} \text{resi}(\text{resi}(A_{1k}, A_{2k}), \text{resi}(A_{1k}, B)) \\ &= A^T \text{resi}(\text{resi}(A_{1k}, A_{2k}), \text{resi}(A_{1k}, B)) = O. \end{aligned} \quad (11)$$

Next, (5) can be rewritten as

$$\text{resi}(\text{resi}(A_{1k}, A_{2k}), \text{resi}(A_{1k}, B)) = B - A \begin{pmatrix} Y - XZ \\ Z \end{pmatrix}.$$

From this and (11), we have

$$A^T \left(B - A \begin{pmatrix} Y - XZ \\ Z \end{pmatrix} \right) = O.$$

Application of Lemma 1 to this proves the lemma. $\square$

QR decomposition and resi have the following relation. Note that QR in this lemma is without pivoting.

Lemma 5 *Let $m \geq n > l$, $A \in \mathbb{R}^{m \times n}$, and $A = QR$ be a QR decomposition partitioned as*

$$A = (A_{1l} \ A_{2l}), \ Q = (Q_{1l} \ Q_{2l}), \ R = \begin{pmatrix} R_{1l} & R_{2l} \\ O & R_{3l} \end{pmatrix}$$

where $A_{1l} \in \mathbb{R}^{m \times l}$, $Q_{1l} \in \mathbb{R}^{m \times l}$, $R_{1l} \in \mathbb{R}^{l \times l}$. If $\text{rank}(A_{1l}) = l$ holds, then

$$\text{resi}(A_{1l}, A_{2l}) = Q_{2l}R_{3l}$$

holds.

Proof We have

$$A_{1l} = Q_{1l}R_{1l}, \ A_{2l} = Q_{1l}R_{2l} + Q_{2l}R_{3l}.$$

Let

$$X = R_{1l}^{-1}R_{2l}.$$

Then, we have

$$Q_{2l}R_{3l} = A_{2l} - A_{1l}X.$$

Furthermore,

$$A_{1l}^T(A_{2l} - A_{1l}X) = A_{1l}^TQ_{2l}R_{3l} = R_{1l}^TQ_{1l}^TQ_{2l}R_{3l} = R_{1l}^TO R_{3l} = O$$

holds. Application of Lemma 1 to this proves the lemma. $\square$

Then, we return to pivoted QR. Let

$$A\Pi_{grd} = (a_{\pi_1} \ a_{\pi_2} \ \dots \ a_{\pi_n}) = (A_{1k} \ A_{2k})$$

where $A_{1k} \in \mathbb{R}^{m \times k}$. From Lemma 5, we can see that

$$\begin{aligned} (1) &\Leftrightarrow \left\| (r_{ll} \ r_{l+1l} \ \dots \ r_{nl})^T \right\|^2 \geq \left\| (r_{lj} \ r_{l+1j} \ \dots \ r_{nj})^T \right\|^2 \\ &\Leftrightarrow \left\| Q_{2(l-1)} (r_{ll} \ r_{l+1l} \ \dots \ r_{nl})^T \right\|^2 \geq \left\| Q_{2(l-1)} (r_{lj} \ r_{l+1j} \ \dots \ r_{nj})^T \right\|^2 \\ &\Leftrightarrow \left\| \text{resi}((a_{\pi_1} \ \dots \ a_{\pi_{l-1}}), a_{\pi_l})^T \right\|^2 \geq \left\| \text{resi}((a_{\pi_1} \ \dots \ a_{\pi_{l-1}}), a_{\pi_j})^T \right\|^2 \end{aligned}$$

for $l = 1, 2, \dots, k$ and $j = l + 1, l + 2, \dots, n$ and

$$\text{pivot}QR_k(A) = \|R_{3k}\|_2 = \|Q_{2k}R_{3k}\|_2 = \|\text{resi}(A_{1k}, A_{2k})\|_2$$

if $\text{rank}(A_{1k}) = k$ holds. The last equation suggests that, as long as $\text{rank}(A_{1k}) = k$ holds, the value of $\text{pivot}QR_k(A)$ is determined only from A_{1k} and A_{2k} , or equivalently from Π_{grd} , and is independent of how (or in what algorithm) the QR decomposition is computed.

3 Evaluation from above

We bound $\frac{\text{pivotQR}_k(A)}{\text{SVD}_k(A)}$ from above in this section. Since $\text{pivotQR}_k(A) = \text{SVD}_k(A) = 0$ holds if $\text{rank}(A) \leq k$ holds, we only consider the case $\text{rank}(A) > k$. Let $A = U\Sigma V^T$ be one SVD. Since $A\Pi_{\text{grd}} = U\Sigma(\Pi_{\text{grd}}^T V)^T$ and $(\Pi_{\text{grd}}^T V)^T(\Pi_{\text{grd}}^T V) = I_n$ hold, $U\Sigma(\Pi_{\text{grd}}^T V)^T$ is one SVD of $A\Pi_{\text{grd}}$. Then, we can see that

$$\text{SVD}_k(A) = \sigma_{k+1}(A) = \sigma_{k+1}(A\Pi_{\text{grd}}).$$

Hereafter, we change what A represents. The previous $A\Pi_{\text{grd}}$ is replaced by A . Let $A \in \mathbb{R}^{m \times n}$ that satisfies

$$\begin{aligned} & \left\| \text{resi}((a_1 \dots a_{i-1}), a_i) \right\| \\ & \geq \left\| \text{resi}((a_1 \dots a_{i-1}), a_j) \right\| \quad (i = 1, \dots, k, j = i + 1, \dots, n) \end{aligned} \quad (12)$$

be partitioned as

$$A = (a_1 \ a_2 \ \dots \ a_n) = (A_{1k} \ A_{2k})$$

where $A_{1k} \in \mathbb{R}^{m \times k}$ and $\text{rank}(A_{1k}) = k$. We should compare $\sigma_{k+1}(A) = \text{SVD}_k(A)$ and $\|\text{resi}(A_{1k}, A_{2k})\|_2 = \text{pivotQR}_k(A)$.

Lemma 6 Let $m \geq n$, $A \in \mathbb{R}^{m \times n}$, and $B \in \mathbb{R}^{m \times l}$. For any $v \in \mathbb{R}^l$,

$$\text{resi}(A, B)v = \text{resi}(A, Bv)$$

holds.

Proof From the definition of resi ,

$$\text{resi}(A, B) = B - AA^\dagger B$$

holds. Thus,

$$\text{resi}(A, B)v = Bv - AA^\dagger Bv = \text{resi}(A, Bv)$$

holds. □

We can see that

$$\begin{aligned} \|\text{resi}(A_{1k}, A_{2k})\|_2 &= \max_{z \in \mathbb{R}^{n-k}, \|z\|=1} \|\text{resi}(A_{1k}, A_{2k})z\| \\ &= \max_{z \in \mathbb{R}^{n-k}, \|z\|=1} \|\text{resi}(A_{1k}, A_{2k}z)\| \end{aligned}$$

from the definition of 2-norm and Lemma 6. Now, we introduce an essential theorem of this paper.

Theorem 2 Let $m \geq n > 1$, $A \in \mathbb{R}^{m \times n}$, $\text{rank}(A) = n$, and A be partitioned as

$$A = (a_1 \ a_2 \ \dots \ a_n).$$

We define $\hat{A}_i$ as

$$\hat{A}_i = (a_1 \ \dots \ a_{i-1} \ a_{i+1} \ \dots \ a_n)$$

for $i = 1, 2, \dots, n$, and d_i as

$$d_i = \text{resi}(\hat{A}_i, a_i)$$

for $i = 1, 2, \dots, n$. Then, $d_i \neq 0$ for $i = 1, 2, \dots, n$ and

$$\frac{\|a_1\|}{\|d_1\|} \leq \sum_{i=2}^n \frac{\|a_i\|}{\|d_i\|}$$

hold.

Proof Since $\text{rank}(A) = n$, $\{a_1, a_2, \dots, a_n\}$ is linearly independent. Because d_i is a linear combination of $\{a_1, a_2, \dots, a_n\}$ with the coefficient of a_i being 1, $d_i \neq 0$ holds for $i = 1, 2, \dots, n$. From the definition of resi ,

$$d_1 = a_1 - \hat{A}_1 x_1$$

holds, where $x_1 = \hat{A}_1^\dagger a_1$. Let $x_1 = (x_{12} \ x_{13} \ \dots \ x_{1n})^T$. Let i be one of $2, 3, \dots, n$. We can see that

$$\|d_i\| \leq \left\| a_i - \hat{A}_i \begin{pmatrix} \frac{1}{x_{1i}} \\ -\frac{x_{1j}}{x_{1i}} \\ -\frac{x_{1j}}{x_{1i}} \\ \vdots \\ -\frac{x_{1j-1}}{x_{1i}} \\ -\frac{x_{1j}}{x_{1i+1}} \\ -\frac{x_{1j}}{x_{1i}} \\ \vdots \\ -\frac{x_{1n}}{x_{1i}} \end{pmatrix} \right\| = \frac{\|d_1\|}{|x_{1i}|}$$

holds if $x_{1i} \neq 0$ from Lemma 3. Thus,

$$|x_{1i}| \leq \frac{\|d_1\|}{\|d_i\|} \quad (13)$$

holds. This (13) also holds if $x_{1i} = 0$. We define $y \in \mathbb{R}^m$ as

$$y = d_1 + x_{1n} a_n = a_1 - \sum_{i=2}^{n-1} x_{1i} a_i.$$

Since $\{\mathbf{a}_1, \mathbf{a}_2, \dots, \mathbf{a}_{n-1}\}$ is linearly independent, $\mathbf{y} \neq \mathbf{0}$ holds. As Lemma 1 gives $\hat{A}_1^T \mathbf{d}_1 = \mathbf{0}$, we have $(\mathbf{a}_n, \mathbf{d}_1) = 0$. Thus,

$$x_{1n} = \frac{(\mathbf{a}_n, \mathbf{y})}{\|\mathbf{a}_n\|^2}$$

holds. We can see that

$$\|\mathbf{d}_n\| \leq \left\| \mathbf{a}_n - \frac{(\mathbf{y}, \mathbf{a}_n)}{\|\mathbf{y}\|^2} \mathbf{y} \right\|$$

holds from Lemma 3 because $\mathbf{y}$ is a linear combination of $\mathbf{a}_i$ ($i = 1, 2, \dots, n-1$). Since

$$\begin{aligned} \|\mathbf{d}_n\|^2 &= \frac{\|\mathbf{d}_n\|^2}{\|\mathbf{d}_1\|^2} \left\| \mathbf{y} - \frac{(\mathbf{a}_n, \mathbf{y})}{\|\mathbf{a}_n\|^2} \mathbf{a}_n \right\|^2 = \frac{\|\mathbf{d}_n\|^2}{\|\mathbf{d}_1\|^2} \|\mathbf{y}\|^2 \left(1 - \frac{(\mathbf{a}_n, \mathbf{y})^2}{\|\mathbf{y}\|^2 \|\mathbf{a}_n\|^2} \right), \\ \left\| \mathbf{a}_n - \frac{(\mathbf{y}, \mathbf{a}_n)}{\|\mathbf{y}\|^2} \mathbf{y} \right\|^2 &= \|\mathbf{a}_n\|^2 \left(1 - \frac{(\mathbf{a}_n, \mathbf{y})^2}{\|\mathbf{y}\|^2 \|\mathbf{a}_n\|^2} \right) \end{aligned}$$

and $\|\mathbf{d}_n\| > 0$ hold,

$$\frac{\|\mathbf{a}_n\|}{\|\mathbf{d}_n\|} \geq \frac{\|\mathbf{y}\|}{\|\mathbf{d}_1\|}$$

holds. Furthermore, since

$$\begin{aligned} \|\mathbf{y}\| &\geq \|\mathbf{a}_1\| - \sum_{i=2}^{n-1} |x_{1i}| \|\mathbf{a}_i\| \\ &\geq \|\mathbf{a}_1\| - \sum_{i=2}^{n-1} \frac{\|\mathbf{d}_i\|}{\|\mathbf{d}_i\|} \|\mathbf{a}_i\| \end{aligned}$$

holds from (13),

$$\frac{\|\mathbf{a}_n\|}{\|\mathbf{d}_n\|} \geq \frac{\|\mathbf{a}_1\|}{\|\mathbf{d}_1\|} - \sum_{i=2}^{n-1} \frac{\|\mathbf{a}_i\|}{\|\mathbf{d}_i\|}$$

holds, and the theorem has been proved. $\square$

We refer to an essential theorem by Hong et al.

Theorem 3 [9, p. 218] Let $m \geq n > l$, $A \in \mathbb{R}^{m \times n}$ and $A = QR = U\Sigma V^T$ be a QR decomposition and an SVD, respectively. Let R and V be partitioned as

$$R = \begin{pmatrix} R_{1l} & R_{2l} \\ O & R_{3l} \end{pmatrix}, \quad V = \begin{pmatrix} V_{1l} & V_{2l} \\ V_{3l} & V_{4l} \end{pmatrix}$$

where $R_{1l} \in \mathbb{R}^{l \times l}$ and $V_{1l} \in \mathbb{R}^{l \times l}$.

$$\|R_{3l}\|_2 \sigma_{n-l}(V_{4l}) \leq \sigma_{l+1}(A)$$

holds.

In the present study, this theorem is only used for $l = n - 1$. The following lemma provides an inequality between resi and the singular value.

Lemma 7 *Under the same assumptions as Theorem 2,*

$$1 \leq (\sigma_n(A))^2 \sum_{i=1}^n \frac{1}{\|\mathbf{d}_i\|^2}$$

holds.

Proof Let $A = U \Sigma V^T$ be an SVD partitioned as

$$V = (V_1 \ \mathbf{v}_2), \ \mathbf{v}_2 = (v_{21} \ v_{22} \ \dots \ v_{2n})^T$$

where $V_1 \in \mathbb{R}^{n \times (n-1)}$. Let $\mathbf{e}_i$ be the i th column of I_n for $i = 1, 2, \dots, n$. Define a permutation matrix Π_i as

$$\Pi_i = (\mathbf{e}_1 \ \dots \ \mathbf{e}_{i-1} \ \mathbf{e}_{i+1} \ \dots \ \mathbf{e}_n \ \mathbf{e}_i)$$

for $i = 1, 2, \dots, n$. Since

$$(\hat{A}_i \ \mathbf{a}_i) = A \Pi_i = U \Sigma (\Pi_i^T V)^T$$

and $(\Pi_i^T V)^T (\Pi_i^T V) = I_n$, $U \Sigma (\Pi_i^T V)^T$ is one SVD of $(\hat{A}_i \ \mathbf{a}_i)$. Let $A \Pi_i = Q_i R_i$ be a QR decomposition partitioned as

$$Q_i = (Q_{i1} \ \mathbf{q}_{i2}), R_i = \begin{pmatrix} R_{i1} & r_{i2} \\ 0 & r_{i3} \end{pmatrix}$$

where $Q_{i1} \in \mathbb{R}^{m \times (n-1)}$, $R_{i1} \in \mathbb{R}^{(n-1) \times (n-1)}$. Using Theorem 3,

$$\sigma_n(A) = \sigma_n(A \Pi_i) \geq |v_{2i}| |r_{i3}|$$

holds. We can see that

$$\|\mathbf{d}_i\| = \|\text{resi}(\hat{A}_i, \mathbf{a}_i)\| = \|r_{i3} \mathbf{q}_{i2}\| = |r_{i3}|$$

holds from Lemma 5. Thus,

$$\sigma_n(A) \geq |v_{2i}| \|\mathbf{d}_i\|$$

holds. Then,

$$1 = \sum_{i=1}^n (v_{2i})^2 \leq (\sigma_n(A))^2 \sum_{i=1}^n \frac{1}{\|d_i\|^2}$$

holds. $\square$

Proposition 2 Let $m \geq n > k$ and $A \in \mathbb{R}^{m \times n}$ satisfy (12) with being partitioned as

$$A = (a_1 \ a_2 \ \dots \ a_n) = (A_{1k} \ A_{2k})$$

where $A_{1k} \in \mathbb{R}^{m \times k}$. Let A satisfy $\text{rank}(A_{1k}) = k$. Then, for all $z \in \mathbb{R}^{n-k}$ with $\|z\| = 1$,

$$\|\text{resi}(A_{1k}, A_{2k}z)\| \leq \sqrt{\frac{4^k - 1}{3}(n - k) + 1} \sigma_{k+1}(A)$$

holds.

Proof From (12) and Lemma 6, the following holds for $i = 1, 2, \dots, k$:

$$\begin{aligned} (n - k) \left\| \text{resi}((a_1 \ \dots \ a_{i-1}), a_i) \right\|^2 &\geq \sum_{j=k+1}^n \left\| \text{resi}((a_1 \ \dots \ a_{i-1}), a_j) \right\|^2 \\ &= \left\| \text{resi}((a_1 \ \dots \ a_{i-1}), A_{2k}) \right\|_F^2 \\ &\geq \left\| \text{resi}((a_1 \ \dots \ a_{i-1}), A_{2k}) \right\|_2^2 \\ &\geq \left\| \text{resi}((a_1 \ \dots \ a_{i-1}), A_{2k}z) \right\|^2. \end{aligned} \quad (14)$$

Define A' as

$$A' = (a_1 \ a_2 \ \dots \ a_k \ A_{2k}z).$$

If $\text{rank}(A') \neq k + 1$, then $\{a_1, a_2, \dots, a_k, A_{2k}z\}$ is linearly dependent. Since

$\text{rank}(A_{1k}) = k$, $\{a_1, a_2, \dots, a_k\}$ is linearly independent, and $A_{2k}z$ can be expressed as a linear combination of $\{a_1, a_2, \dots, a_k\}$. Then, we have

$\text{resi}(A_{1k}, A_{2k}z) = \mathbf{0}$ from Lemma 3, and the conclusion holds. Therefore, we only consider the case $\text{rank}(A') = k + 1$ in the remainder of this proof. We define d'_i as

$$d'_i = \text{resi}((a_1 \ \dots \ a_{i-1} \ a_{i+1} \ \dots \ a_k \ A_{2k}z), a_i) \ (i = 1, 2, \dots, k).$$

From Lemma 4, we can see that

$$d'_j = \text{resi}\left(\text{resi}((a_1 \ \dots \ a_{i-1}), A'_{ijk}), \text{resi}((a_1 \ \dots \ a_{i-1}), a_j)\right)$$

holds for $i = 1, 2, \dots, k$ and $j = i, i + 1, \dots, k$, where

$$A'_{ijk} = (a_i \ \dots \ a_{j-1} \ a_{j+1} \ \dots \ a_k \ A_{2k}z), \text{ and}$$

$$\begin{aligned} & \text{resi}(A_{1k}, A_{2k}z) \\ &= \text{resi}(\text{resi}((a_1 \dots a_{i-1}), (a_i \dots a_k)), \text{resi}((a_1 \dots a_{i-1}), A_{2k}z)) \end{aligned}$$

holds for $i = 1, 2, \dots, k$. Using Theorem 2 on $\text{resi}((a_1 \ a_2 \dots a_{i-1}), (a_i \ a_{i+1} \dots a_k \ A_{2k}z))$, we can see that

$$\begin{aligned} & \frac{\|\text{resi}((a_1 \ a_2 \dots a_{i-1}), a_i)\|}{\|\text{resi}(\text{resi}((a_1 \dots a_{i-1}), A'_{iik}), \text{resi}((a_1 \dots a_{i-1}), a_i))\|} \\ & \leq \sum_{j=i+1}^k \frac{\|\text{resi}((a_1 \ a_2 \dots a_{i-1}), a_j)\|}{\|\text{resi}(\text{resi}((a_1 \dots a_{i-1}), A'_{ijk}), \text{resi}((a_1 \dots a_{i-1}), a_j))\|} \\ & \quad + \frac{\|\text{resi}((a_1 \ a_2 \dots a_{i-1}), A_{2k}z)\|}{\|\text{resi}(\text{resi}((a_1 \dots a_{i-1}), (a_i \dots a_k)), \text{resi}((a_1 \dots a_{i-1}), A_{2k}z))\|} \end{aligned}$$

holds. Thus,

$$\begin{aligned} & \frac{\|\text{resi}((a_1 \ a_2 \dots a_{i-1}), a_i)\|}{\|d'_i\|} \\ & \leq \sum_{j=i+1}^k \frac{\|\text{resi}((a_1 \ a_2 \dots a_{i-1}), a_j)\|}{\|d'_j\|} + \frac{\|\text{resi}((a_1 \ a_2 \dots a_{i-1}), A_{2k}z)\|}{\|\text{resi}(A_{1k}, A_{2k}z)\|} \\ & \leq \|\text{resi}((a_1 \ a_2 \dots a_{i-1}), a_i)\| \left(\sum_{j=i+1}^k \frac{1}{\|d'_j\|} + \frac{\sqrt{n-k}}{\|\text{resi}(A_{1k}, A_{2k}z)\|} \right) \end{aligned}$$

holds for $i = 1, 2, \dots, k$ from (12) and (14). Thus,

$$\frac{1}{\|d'_i\|} \leq \sum_{j=i+1}^k \frac{1}{\|d'_j\|} + \frac{\sqrt{n-k}}{\|\text{resi}(A_{1k}, A_{2k}z)\|} \quad (i = 1, 2, \dots, k) \quad (15)$$

holds. We want to show that

$$\frac{1}{\|d'_i\|} \leq \frac{2^{k-i}\sqrt{n-k}}{\|\text{resi}(A_{1k}, A_{2k}z)\|} \quad (i = 1, 2, \dots, k) \quad (16)$$

and prove this using induction in the order of $i = k, k-1, \dots, 1$. Applying (15) for $i = k$ gives

$$\frac{1}{\|d'_k\|} \leq \frac{\sqrt{n-k}}{\|\text{resi}(A_{1k}, A_{2k}z)\|} = \frac{2^{k-k}\sqrt{n-k}}{\|\text{resi}(A_{1k}, A_{2k}z)\|}.$$

Thus, (16) is shown in case $i = k$. Then, we prove that (16) holds for $i = l$, assuming that (16) holds for $i = l + 1, l + 2, \dots, k$. We can see that

$$\begin{aligned} \frac{1}{\|d'_l\|} &\leq \sum_{j=l+1}^k \frac{1}{\|d'_j\|} + \frac{\sqrt{n-k}}{\|\text{resi}(A_{1k}, A_{2k}z)\|} \\ &\leq \frac{\sqrt{n-k}}{\|\text{resi}(A_{1k}, A_{2k}z)\|} \left(\sum_{j=l+1}^k 2^{k-j} + 1 \right) \\ &= \frac{2^{k-l} \sqrt{n-k}}{\|\text{resi}(A_{1k}, A_{2k}z)\|} \end{aligned}$$

holds from (15) and the assumption of induction. Thus, (16) has been shown in case $i = 1, 2, \dots, k$. Using Lemma 7 on A' ,

$$\begin{aligned} 1 &\leq (\sigma_{k+1}(A'))^2 \left(\sum_{i=1}^k \frac{1}{\|d'_i\|^2} + \frac{1}{\|\text{resi}(A_{1k}, A_{2k}z)\|^2} \right) \\ &\leq \frac{(\sigma_{k+1}(A'))^2}{\|\text{resi}(A_{1k}, A_{2k}z)\|^2} \left((n-k) \sum_{i=1}^k 4^{k-i} + 1 \right) \\ &= \frac{(\sigma_{k+1}(A'))^2}{\|\text{resi}(A_{1k}, A_{2k}z)\|^2} \left(\frac{4^k - 1}{3} (n-k) + 1 \right) \end{aligned}$$

holds. Thus,

$$\|\text{resi}(A_{1k}, A_{2k}z)\| \leq \sqrt{\frac{4^k - 1}{3} (n-k) + 1} \sigma_{k+1}(A')$$

holds. Now, if we can show that

$$\sigma_{k+1}(A') \leq \sigma_{k+1}(A),$$

then the proof is complete. Considering the fact that

$$\sigma_{k+1}(A) = \max_{\Theta, \dim \Theta = k+1} \min_{x \in \Theta, \|x\|=1} \|Ax\|,$$

we want a subspace Θ that satisfies

$$\min_{x \in \Theta, \|x\|=1} \|Ax\| \geq \sigma_{k+1}(A').$$

Let

$$\Theta' = \text{span} \left\{ e_1, e_2, \dots, e_k, \begin{pmatrix} \mathbf{0} \\ z \end{pmatrix} \right\}.$$

Then, we have $\dim(\Theta') = k + 1$ since $\left\{e_1, e_2, \dots, e_k, \begin{pmatrix} \mathbf{0} \\ z \end{pmatrix}\right\}$ is linearly independent. Let $y = (y_i) \in \mathbb{R}^{k+1}$. Since $\begin{pmatrix} e_1 & e_2 & \dots & e_k & \begin{pmatrix} \mathbf{0} \\ z \end{pmatrix} \end{pmatrix}^T \begin{pmatrix} e_1 & e_2 & \dots & e_k & \begin{pmatrix} \mathbf{0} \\ z \end{pmatrix} \end{pmatrix} = I_{k+1}$ holds,

$$\|y\| = 1 \Leftrightarrow \left\| \sum_{i=1}^k y_i e_i + y_{k+1} \begin{pmatrix} \mathbf{0} \\ z \end{pmatrix} \right\| = 1 \quad (17)$$

holds. For all $y \in \mathbb{R}^{k+1}$ that satisfies the right-hand side of (17),

$$\left\| A \left(\sum_{i=1}^k y_i e_i + y_{k+1} \begin{pmatrix} \mathbf{0} \\ z \end{pmatrix} \right) \right\| = \|A'y\| \geq \sigma_{k+1}(A')$$

holds. Then,

$$\sigma_{k+1}(A) \geq \min_{x \in \Theta', \|x\|=1} \|Ax\| \geq \sigma_{k+1}(A')$$

holds. $\square$

Thus, we have proved that

$$\text{pivotQR}_k(A) \leq \sqrt{\frac{4^k - 1}{3}(n - k) + 1} \text{SVD}_k(A).$$

4 Evaluation from below

In this section, we show that the inequality proved in the previous section is tight. An example of matrix R_h with real-valued parameter h that satisfies

$$\frac{\text{pivotQR}_k(R_h)}{\text{SVD}_k(R_h)} \xrightarrow{h \rightarrow 0} \sqrt{\frac{4^k - 1}{3}(n - k) + 1}$$

is shown. R_h is as follows:

$$R_h = \begin{pmatrix} 1 & 0 & \dots & 0 \\ 0 & h & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \dots & 0 & h^k \\ & & O & \end{pmatrix} O \begin{pmatrix} 1 & -\sqrt{1-h^2} & \dots & -\sqrt{1-h^2} & \dots & -\sqrt{1-h^2} \\ 0 & 1 & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & -\sqrt{1-h^2} & \dots & -\sqrt{1-h^2} \\ 0 & \dots & 0 & 1 & \dots & 1 \\ & & O & & & \end{pmatrix}.$$

The Kahan matrix is [10]

$$K_n = \begin{pmatrix} 1 & 0 & \dots & 0 \\ 0 & h & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \dots & 0 & h^{n-1} \end{pmatrix} \begin{pmatrix} 1 & -\sqrt{1-h^2} & \dots & -\sqrt{1-h^2} \\ 0 & 1 & \ddots & \vdots \\ \vdots & \ddots & \ddots & -\sqrt{1-h^2} \\ 0 & \dots & 0 & 1 \end{pmatrix}.$$

Therefore, R_h is the same as the Kahan matrix in case $m = n = k + 1$ and is an extension of the Kahan matrix otherwise.

Proposition 3 Let $m \geq n > k$. Define $\Sigma_h \in \mathbb{R}^{m \times n}$, $(w_{hij}) = W_h \in \mathbb{R}^{n \times n}$, and $R_h \in \mathbb{R}^{m \times n}$ as follows:

$$\Sigma_h = \begin{pmatrix} \text{diag}(1, h, \dots, h^k, 0, 0, \dots, 0) \\ O \end{pmatrix},$$

$$w_{hij} = \begin{cases} 1 & (i = j \text{ and } 1 \leq i \leq k) \text{ or } (i = k + 1 \text{ and } k + 1 \leq j \leq n), \\ -\sqrt{1-h^2} & (i < j \text{ and } 1 \leq i \leq k), \\ 0 & \text{otherwise} \end{cases}$$

and $R_h = \Sigma_h W_h$ where $0 < h < 1$. Then,

$$\lim_{h \rightarrow 0} \frac{\text{pivotQR}_k(R_h)}{\text{SVD}_k(R_h)} = \sqrt{\frac{4^k - 1}{3}(n - k) + 1}$$

holds.

Proof Let $Q = \begin{pmatrix} I_n \\ O \end{pmatrix} \in \mathbb{R}^{m \times n}$ and $R = \text{diag}(1, h, \dots, h^k, 0, 0, \dots, 0)W_h \in \mathbb{R}^{n \times n}$. Since R is an upper triangular matrix and $Q^T Q = I_n$ holds, $R_h = QR$ is one QR decomposition. We check (1) for this R . Since

$$\begin{aligned} (\text{left side of (1)}) &= h^{2l-2} = (1-h^2) \sum_{i=l}^{\min(j,k+1)-1} h^{2i-2} + h^{2\min(j,k+1)-2} \\ &= (\text{right side of (1)}), \end{aligned}$$

(1) holds for $l = 1, 2, \dots, k + 1$, $j = l + 1, l + 2, \dots, n$. Obviously (1) also holds for $l = k + 2, k + 3, \dots, n - 1$, $j = l + 1, l + 2, \dots, n$. As in Sect. 2, let R be partitioned as

$$R = \begin{pmatrix} R_{1k} & R_{2k} \\ O & R_{3k} \end{pmatrix}$$

where $R_{1k} \in \mathbb{R}^{k \times k}$. Then,

$$\text{pivotQR}_k(R_h) = \|R_{3k}\|_2$$

holds. Define $V \in \mathbb{R}^{(n-k) \times (n-k)}$ and $\mathbf{v}_1 \in \mathbb{R}^{n-k}$ as follows:

$$V = (\mathbf{v}_1 \ \mathbf{v}_2 \ \dots \ \mathbf{v}_{n-k}), \quad \mathbf{v}_1 = \frac{1}{\sqrt{n-k}} (1 \ 1 \ \dots \ 1)^T$$

where $\mathbf{v}_2, \mathbf{v}_3, \dots, \mathbf{v}_{n-k}$ are chosen such that $V^T V = I_{n-k}$ holds. We can choose them freely as long as this is satisfied. Since

$$R_{3k} = h^k \sqrt{n-k} (\mathbf{v}_1 \ \mathbf{0} \ \dots \ \mathbf{0})^T$$

holds, $\|R_{3k}\|_2 = h^k \sqrt{n-k}$ holds. We consider the value of $SVD_k(R_h) = \sigma_{k+1}(R_h)$. Considering the fact that

$$\sigma_{k+1}(R_h) = \min_{\Theta, \dim \Theta = n-k} \max_{\mathbf{x} \in \Theta, \|\mathbf{x}\|=1} \|R_h \mathbf{x}\|,$$

we want a subspace Θ whose $\max_{\mathbf{x} \in \Theta, \|\mathbf{x}\|=1} \|R_h \mathbf{x}\|$ is small. Since $\mathbf{v}_1^T \mathbf{v}_i = 0$ holds for $i = 2, 3, \dots, n-k$,

$$R_h \begin{pmatrix} \mathbf{0} \\ \mathbf{v}_i \end{pmatrix} = \begin{pmatrix} R_{2k} \\ R_{3k} \\ O \end{pmatrix} \mathbf{v}_i = \begin{pmatrix} -\sqrt{(n-k)(1-h^2)} h^0 \\ -\sqrt{(n-k)(1-h^2)} h^1 \\ \vdots \\ -\sqrt{(n-k)(1-h^2)} h^{k-1} \\ \sqrt{n-k} h^k \\ 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix} \mathbf{v}_1^T \mathbf{v}_i = \mathbf{0}$$

holds for $i = 2, 3, \dots, n-k$. We define $y_j = 1$ for $j = k+1, \dots, n$ and define y_j from $j = k$ down to $j = 1$ as $y_j = \sqrt{1-h^2} \sum_{i=j+1}^n y_i$. We define $\mathbf{y} \in \mathbb{R}^n$ as $(y_1 \ y_2 \ \dots \ y_n)^T$. Then,

$$R_h \mathbf{y} = (0 \ 0 \ \dots \ 0 \ (n-k)h^k \ 0 \ 0 \ \dots \ 0)^T$$

holds. Since

$$\begin{aligned} \lim_{h \rightarrow 0} \|\mathbf{y}\| &= \left\| \begin{pmatrix} (n-k)2^{k-1} & (n-k)2^{k-2} & \dots & (n-k)2^0 & 1 & 1 & \dots & 1 \end{pmatrix} \right\| \\ &= \sqrt{\frac{4^k - 1}{3} (n-k)^2 + n - k} \end{aligned}$$

holds,

$$\lim_{h \rightarrow 0} \frac{1}{h^k} \left\| R_h \frac{\mathbf{y}}{\|\mathbf{y}\|} \right\| = \frac{\sqrt{n-k}}{\sqrt{\frac{4^k-1}{3}(n-k)+1}}$$

holds. Let

$$\Theta' = \text{span} \left\{ \frac{\mathbf{y}}{\|\mathbf{y}\|}, \begin{pmatrix} \mathbf{0} \\ \mathbf{v}_2 \end{pmatrix}, \begin{pmatrix} \mathbf{0} \\ \mathbf{v}_3 \end{pmatrix}, \dots, \begin{pmatrix} \mathbf{0} \\ \mathbf{v}_{n-k} \end{pmatrix} \right\}.$$

Then, we have $\dim(\Theta') = n - k$. Since

$$\begin{pmatrix} \frac{\mathbf{y}}{\|\mathbf{y}\|} & \begin{pmatrix} \mathbf{0} \\ \mathbf{v}_2 \end{pmatrix} & \begin{pmatrix} \mathbf{0} \\ \mathbf{v}_3 \end{pmatrix} & \cdots & \begin{pmatrix} \mathbf{0} \\ \mathbf{v}_{n-k} \end{pmatrix} \end{pmatrix}^T \begin{pmatrix} \frac{\mathbf{y}}{\|\mathbf{y}\|} & \begin{pmatrix} \mathbf{0} \\ \mathbf{v}_2 \end{pmatrix} & \begin{pmatrix} \mathbf{0} \\ \mathbf{v}_3 \end{pmatrix} & \cdots & \begin{pmatrix} \mathbf{0} \\ \mathbf{v}_{n-k} \end{pmatrix} \end{pmatrix} \\ = I_{n-k}$$

holds, we have

$$\sum_{i=1}^{n-k} z_i^2 = 1 \Leftrightarrow \left\| z_1 \frac{\mathbf{y}}{\|\mathbf{y}\|} + \sum_{i=2}^{n-k} z_i \begin{pmatrix} \mathbf{0} \\ \mathbf{v}_i \end{pmatrix} \right\| = 1 \quad (18)$$

for $z_1, z_2, \dots, z_{n-k} \in \mathbb{R}$. Thus, if the right-hand side of (18) holds, we have

$$\begin{aligned} & \left\| \frac{1}{h^k} R_h \left(z_1 \frac{\mathbf{y}}{\|\mathbf{y}\|} + \sum_{i=2}^{n-k} z_i \begin{pmatrix} \mathbf{0} \\ \mathbf{v}_i \end{pmatrix} \right) \right\| \\ &= \frac{|z_1|}{h^k} \left\| R_h \frac{\mathbf{y}}{\|\mathbf{y}\|} \right\| \leq \frac{1}{h^k} \left\| R_h \frac{\mathbf{y}}{\|\mathbf{y}\|} \right\| \xrightarrow{h \rightarrow 0} \frac{\sqrt{n-k}}{\sqrt{\frac{4^k-1}{3}(n-k)+1}}. \end{aligned}$$

Then, we have

$$\lim_{h \rightarrow 0} \frac{\sigma_{k+1}(R_h)}{h^k} \leq \lim_{h \rightarrow 0} \frac{1}{h^k} \max_{x \in \Theta', \|x\|=1} \|R_h x\| \leq \frac{\sqrt{n-k}}{\sqrt{\frac{4^k-1}{3}(n-k)+1}}.$$

Thus,

$$\lim_{h \rightarrow 0} \frac{\text{pivotQR}_k(R_h)}{\text{SVD}_k(R_h)} \geq \sqrt{\frac{4^k-1}{3}(n-k)+1}$$

holds, and the theorem has been proved using the results of the previous section. $\square$

5 Numerical experiments

5.1 Experiments

Because $SVD_k(R_h)$ cannot be calculated numerically when h is very small, we prepare another matrix for the experiments. Here, we present the matrix in case $k = n - 1$.

Proposition 4 [11] *Let $m \geq n$ and $\epsilon_i \in \mathbb{R}$ satisfy $0 < \epsilon_i < 1$ ($i = 1, 2, \dots, n$). Let $\{\mathbf{v}_i\}_{i=1}^n \in \mathbb{R}^n$ be*

$$v_{j,i} = \begin{cases} 0 & (j < i) \\ -1 - \epsilon_i & (j = i) \\ 1 - \epsilon_i & (j > i) \end{cases}$$

where $v_{j,i}$ is the j -th element of $\mathbf{v}_i$. Let $\{\mathbf{w}_i\}_{i=1}^n$ be the output of performing the Gram-Schmidt orthonormalization on $\{\mathbf{v}_i\}_{i=1}^n$. Define $\Sigma \in \mathbb{R}^{m \times n}$ and $W \in \mathbb{R}^{n \times n}$ as follows:

$$\Sigma = \begin{pmatrix} \text{diag}(\sigma_1, \sigma_2, \dots, \sigma_n) \\ O \end{pmatrix},$$

$$W = (\mathbf{w}_1 \ \mathbf{w}_2 \ \dots \ \mathbf{w}_n),$$

where $\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_n > 0$. Let $A = \Sigma W^T$. Then,

$$\lim_{(\epsilon_1, \epsilon_2, \dots, \epsilon_n) \rightarrow (0, \dots, 0)} \lim_{\sigma_{n-1} \rightarrow \infty} \lim_{\sigma_{n-2} \rightarrow \infty} \dots \lim_{\sigma_1 \rightarrow \infty} \frac{\text{pivotQR}_{n-1}(A)}{SVD_{n-1}(A)} = \sqrt{\frac{4^{n-1} + 2}{3}}$$

holds.

This proposition introduces matrices that converge to the least upper bound only in case $k = n - 1$. In this paper, matrices that conjecturally converge to the least upper bound in case $k < n - 1$ are defined in an analogous manner as follows.

Conjecture 1 *Let $m \geq n > k$ and $\epsilon_i \in \mathbb{R}$ satisfy $0 < \epsilon_i < 1$ ($i = 1, 2, \dots, n$). Let $\{\mathbf{v}_i\}_{i=1}^n \in \mathbb{R}^n$ be*

$$v_{j,i} = \begin{cases} -1 - \epsilon_i & (j = i) \text{ or } ((i = k + 1) \text{ and } (k + 1 \leq j)) \\ 1 - \epsilon_i & (j > i) \text{ and } (i \leq k) \\ 0 & (\text{otherwise}) \end{cases}$$

where $v_{j,i}$ is the j -th element of $\mathbf{v}_i$. Let $\{\mathbf{w}_i\}_{i=1}^n$ be the output of performing the Gram-Schmidt orthonormalization on $\{\mathbf{v}_i\}_{i=1}^n$. Define $\Sigma \in \mathbb{R}^{m \times n}$ and $W \in \mathbb{R}^{n \times n}$ as follows:

$$\Sigma = \begin{pmatrix} \text{diag}(\sigma_1, \dots, \sigma_{k+1}, 0, \dots, 0) \\ O \end{pmatrix},$$

$$W = (\mathbf{w}_1 \ \mathbf{w}_2 \ \dots \ \mathbf{w}_n),$$

where $\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_{k+1} > 0$. Let $A = \Sigma W^T$. Then,

$$\lim_{(\epsilon_1, \epsilon_2, \dots, \epsilon_n) \rightarrow (0, \dots, 0)} \lim_{\sigma_k \rightarrow \infty} \lim_{\sigma_{k-1} \rightarrow \infty} \dots \lim_{\sigma_1 \rightarrow \infty} \frac{\text{pivotQR}_k(A)}{\text{SVD}_k(A)} = \sqrt{\frac{4^k - 1}{3}(n - k) + 1}$$

holds. $\square$

$\{\mathbf{v}_i\}_{i=1}^n$ is as follows:

$$(\mathbf{v}_1 \ \mathbf{v}_2 \ \dots \ \mathbf{v}_n) = \begin{pmatrix} -1 - \epsilon_1 & 1 - \epsilon_1 & \dots & \dots & 1 - \epsilon_1 & \dots & 1 - \epsilon_1 \\ 0 & -1 - \epsilon_2 & 1 - \epsilon_2 & \dots & 1 - \epsilon_2 & \dots & 1 - \epsilon_2 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \\ \vdots & \ddots & \ddots & -1 - \epsilon_k & 1 - \epsilon_k & \dots & 1 - \epsilon_k \\ \vdots & \ddots & \ddots & 0 & -1 - \epsilon_{k+1} & \dots & -1 - \epsilon_{k+1} \\ \vdots & \ddots & \ddots & 0 & 0 & \ddots & 0 \\ 0 & \ddots & \ddots & 0 & 0 & 0 & -1 - \epsilon_n \end{pmatrix}.$$

Fig. 1 $s = 10^9, \mu = \frac{\sqrt{\frac{4^k - 1}{3}(n - k) + 1}}{\frac{\text{pivotQR}_k(A)}{\text{SVD}_k(A)}} - 1$

Fig. 2 $n = 25, u = \frac{\sqrt{\frac{4^k-1}{3}(n-k)+1}}{\frac{\text{pivotQR}_k(A)}{\text{SVD}_k(A)}} - 1$

Because the limits cannot be taken in numerical experiments, we assign s^{n-i} to σ_i for $i = 1, 2, \dots, k+1$ and s^{-1} to ϵ_i for $i = 1, 2, \dots, n$. Numerical experiments were performed for $n = 2, 3, \dots, 25$ and $k = 1, 2, \dots, n-1$ with $m = n$. We calculate u as follows:

$$u = \frac{\sqrt{\frac{4^k-1}{3}(n-k)+1}}{\frac{\text{pivotQR}_k(A)}{\text{SVD}_k(A)}} - 1.$$

Because we want $\frac{\text{pivotQR}_k(A)}{\text{SVD}_k(A)} \rightarrow \sqrt{\frac{4^k-1}{3}(n-k)+1}$ as $s \rightarrow \infty$, we want $u \rightarrow 0$ as $s \rightarrow \infty$.

5.2 Environment

Python 3.5.2, scipy 1.4.1, and numpy 1.13.3 were used. The data type used in these experiments was double precision. We used SVD of numpy and pivoted QR of scipy. Gram-Schmidt orthonormalization was performed twice using the scipy QR decomposition. Let $V = (v_1 \dots v_n)$ and $V = QR$ and $Q = WR'$ be QR decompositions. The i -th column of W is assigned to w_i for $i = 1, 2, \dots, n$.

5.3 Results

The maximum value of u is $2.3482077194 \cdot 10^{-5}$ and $u \geq 0$ holds in all cases where $s = 10^9$. The results of cases $m = n = 2, 3, \dots, 25$, $k = n - 1$, $\lfloor \frac{n}{2} \rfloor$, $\lfloor \log_2 n \rfloor$, and $s = 10^9$ are shown in Fig. 1. We can see that it almost approaches the least upper bound, and u increases monotonically with n and k . The results of cases $m = n = 25$, $k = n - 1, \lfloor \frac{n}{2} \rfloor, \lfloor \log_2 n \rfloor$, and $s = 10, 10^2, \dots, 10^9$ are shown in Fig. 2. We can see that u decreases monotonically with s . From these results, we can see that numerical solutions are likely to converge to the least upper bound.

6 Conclusion

We compare the 2-norm of the truncation error of pivoted QR to that of SVD. We obtain the following theorem:

Theorem 4 *Let $m \geq n > k$. For any $A \in \mathbb{R}^{m \times n}$,*

$$\text{pivotQR}_k(A) \leq \sqrt{\frac{4^k - 1}{3}(n - k) + 1} \text{SVD}_k(A)$$

holds. Furthermore, for $t \in \mathbb{R}$ that satisfies $t < \sqrt{\frac{4^k - 1}{3}(n - k) + 1}$, there exists $A \in \mathbb{R}^{m \times n}$ that satisfies

$$\text{pivotQR}_k(A) > t \text{SVD}_k(A).$$

□

This proposition states that the least upper bound of the ratio of the truncation error of pivoted QR to that of SVD is $\sqrt{\frac{4^k - 1}{3}(n - k) + 1}$ when an $m \times n$ ($m \geq n$) matrix is approximated to a matrix whose rank is k . Furthermore, an example where the ratio converges to the least upper bound is found. We also find an example where the ratio is close to the least upper bound through a numerical experiment in case n is small.

7 Future work

We can see that the least upper bound of the ratio of the truncation error of pivoted QR to that of SVD is $O(2^k \sqrt{n})$. However, this upper bound is attained only on a contrived example [4]. We expect that the upper bound may become significantly smaller by adding some restrictions to the matrices. We intend to find such a property.

Open Access This article is licensed under a Creative Commons Attribution 4.0 International License, which permits use, sharing, adaptation, distribution and reproduction in any medium or format, as long as you give appropriate credit to the original author(s) and the source, provide a link to the Creative Commons licence, and indicate if changes were made. The images or other third party material in this article are included in the article's Creative Commons licence, unless indicated otherwise in a credit line to the material. If material is not included in the article's Creative Commons licence and your intended use is not permitted by statutory regulation or exceeds the permitted use, you will need to obtain permission directly from the copyright holder. To view a copy of this licence, visit <http://creativecommons.org/licenses/by/4.0/>.

References

1. Björck, Å.: Numerical Methods for Least Squares Problems. SIAM, Philadelphia (1996)
2. Businger, P., Golub, G.H.: Linear least squares solutions by householder transformations. *Numer. Math.* **7**, 269–276 (1965)
3. Chandrasekaran, S., Ipsen, I.C.F.: On rank-revealing factorisations. *SIAM J. Matrix Anal. Appl.* **15**(2), 592–622 (1994)
4. Drmač, Z., Gugercin, S.: A new selection operator for the discrete empirical interpolation method-improved a priori error bound and extensions. *SIAM J. Sci. Comput.* **38**(2), A631–A648 (2016)
5. Eldén, L.: Numerical linear algebra in data mining. *Acta Numer.* **15**, 327–384 (2006)
6. Faddeev, D.K., Kublanovskaya, V.N., Faddeeva, V.N.: Solution of linear algebraic systems with rectangular matrices. *Trudy Mat. Inst. Steklov.* **96**, 76–92 (1968)
7. Golub, G.H.: Numerical methods for solving linear least squares problems. *Numer. Math.* **7**, 206–216 (1965)
8. Golub, G.H., Van Loan, C.F.: Matrix Computations, 3rd edn. The Johns Hopkins University Press, Baltimore (1996)
9. Hong, Y.P., Pan, C.-T.: Rank-revealing QR factorizations and the singular value decomposition. *Math. Comput.* **58**, 213–232 (1992)
10. Kahan, W.: Numerical linear algebra. *Can. Math. Bull.* **9**, 757–801 (1966)
11. Kawamura, H.: Analysis of truncation error of matrix low rank approximation algorithm using QR decomposition with pivot selection. *Trans. Jpn. Soc. Ind. Appl. Math.* **30**(2), 163–176 (2020)
12. Khoromskij, B.N.: Tensors-structured numerical methods in scientific computing: survey on recent advances. *Chemom. Intell. Lab. Syst.* **110**, 1–19 (2012)
13. Kumar, N.K., Schneider, J.: Literature survey on low rank approximation of matrices. *Linear Multilinear Algebra* **65**(11), 2212–2244 (2017)
14. Ye, J.: Generalized low rank approximations of matrices. *Mach. Learn.* **61**, 167–191 (2005)

Publisher's Note Springer Nature remains neutral with regard to jurisdictional claims in published maps and institutional affiliations.