

Numerical Properties of Preconditioning in the One-Sided Block-Jacobi SVD Algorithm

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Abstract. We analyze the numerical properties of the preconditioning of type AV (or VA) for the subsequent singular value decomposition of a matrix $A \in \mathbb{R}^{m \times n}$, $m \geq n$, using the one-sided Jacobi algorithm. The analysis is performed in floating point arithmetic with the round-off unit u . When $A = BD$ (or $A = DB$) with B well-conditioned with columns of unit Euclidean norm and D diagonal (or D diagonal and B well-conditioned with rows of unit Euclidean norm), it is shown that for an orthogonal or numerically orthogonal matrix V all singular triplets of the computed matrix $\hat{C} = fl(VA)$ (or $\hat{C} = fl(AV)$) are only small relative perturbations of the singular triplets of a matrix A . Moreover, when a numerically orthogonal matrix V is close to the matrix of right singular vectors of A , the upper bound for the loss of orthogonality in columns of $\hat{C}$ is provided, which is proportional to the 2-norm condition number $\kappa_2(A)$. Numerical examples in MATLAB illustrate the theoretical results.

Keywords: preconditioning, polar decomposition, Halley's iterations, loss of orthogonality, one-sided block-Jacobi algorithm

1 Introduction

In [1], we have proposed the use of the (partial) polar decomposition (PD) for the preconditioning of the one-sided block-Jacobi algorithm (OSBJA) for the singular value decomposition (SVD) of a given matrix $A \in \mathbb{R}^{m \times n}$, $m \geq n$, of full column rank. The preconditioner comes from the eigenvalue decomposition (EVD) of the symmetric, positive semi-definite factor H of order n , which is computed by using (partial) Halley's iterations that converge cubically. Hence, the numerically orthogonal matrix V of eigenvectors of H is used for the preconditioning $C = AV$, and the OSBJA is applied to matrix C . This approach eliminates the computation of the Gram matrix $fl(A^T A)$, which is not numerically reliable for very ill-conditioned matrices A .

Note that when $A = UH$ is the polar decomposition of A , $H = VAV^T$ is the EVD of H and $A = P\Sigma S^T$ is the SVD of A , then $AV = (UV)A$ so that

$P = UV$, $\Sigma = \Lambda$ and $S = V$. In other words, in exact arithmetic the matrix V is the matrix of right singular vectors of A , $P = UV$ is the matrix of left singular vectors, and the OSBJA applied to $C = AV$ converges to the matrix $(UV)\Lambda = P\Sigma$, i.e. to the column-scaled matrix of left singular vectors of A .

It is well known (see [2]), that for *column-graded* matrices of the form $A = BD$, where B is well-conditioned with columns of unit Euclidean norm and D is diagonal with norms of columns of A on diagonal and possibly very ill-conditioned, the element-wise one-sided Jacobi SVD algorithm (applied from the right or left) delivers *all* singular triplets with high relative accuracy (regardless of conditioning of D and therefore also of A). In fact, it is the unique known algorithm with such a property. Note that when $A = BD$, the preconditioned matrix $AV = BDV$ is *not* column-graded anymore. Hence, for column-graded matrices it is better to use the preconditioning from the left, $\tilde{V}A = \tilde{V}BD$, which preserves the grading. This means that one needs to compute the polar decomposition of A^T instead of A : $A^T = \tilde{U}\tilde{H}$, and the EVD of the symmetric, positive semi-definite $\tilde{H}$: $\tilde{H} = Q\tilde{\Lambda}Q^T$. Then:

$$A = \tilde{H}\tilde{U}^T = Q\tilde{\Lambda}(\tilde{U}Q)^T,$$

so that one has for the SVD of $A = P\Sigma S^T$: $P = Q$, $\Sigma = \tilde{\Lambda}$, $S = \tilde{U}Q$. Using $\tilde{V} = Q^T$ in the preconditioning, the OSBJA applied to $\tilde{V}A = Q^T A$ converges to the column-scaled, transposed matrix of right singular vectors $(S\Sigma)^T = (\tilde{U}Q A)^T$.

In the following, we wish to preserve the grading of matrix A , so we will apply our preconditioner V from the left, and the OSBJA will be applied to VA . Note that for row-graded matrices $A = DB$, B well-conditioned with unit rows and D diagonal, the original preconditioning AV from the right described in [1] preserves the row grading. In the following, we consider matrices of the form $A = BD$ with the preconditioning VA , but our results are applicable (with proper modifications) also for matrices of the form $A = DB$ with the preconditioning AV .

All relations above are valid in exact arithmetic. But in real life, all computations are performed in the floating point arithmetic with the round-off unit $\mathbf{u}$. Since our preconditioning has the form of matrix-matrix multiplication in floating point arithmetic, and we wish to compute the SVD of the original matrix A , we have to analyze first the perturbations of singular triplets $(p_i, \sigma_i(A), s_i)$, $1 \leq i \leq n$, of matrix A after its multiplication by $\hat{V}$, i.e. after computing $\hat{C} = \hat{V}A$, where $\hat{V}$ is only numerically orthogonal. After listing the known results in Section 2, the perturbation analysis is done in Section 3.

When a numerically orthogonal matrix $\hat{V}$ is close to the matrix of right singular vectors of A , the upper bound for the loss of orthogonality in columns of $C = A\hat{V}$ is derived using exact arithmetic in Section 4, which is proportional to the 2-norm condition number $\kappa_2(A)$. Such a matrix $\hat{V}$ is computed, for example, as the eigenvector matrix of the Hermitian factor arising from the (partial) polar decomposition of A using cubically convergent Halley's iterations (see [1]). In Section 5, numerical experiments computed in MATLAB illustrate the theoretical results, and the paper ends with some conclusions.

2 Preliminaries

This section summarizes main known results that are used in our perturbation analysis. They are presented without proofs that can be found in the cited literature.

In the following, the symbols $\|X\|_2$ and $\|X\|_F$ denote the 2-norm and the Frobenius norm, respectively, of a matrix X , $\kappa_2(X)$ is its 2-norm condition number and $\|y\|_2$ denotes the Euclidean norm of a vector y .

We start with the general theorem about the relative error in *all* singular values of matrix A after its small additive perturbation δA . Note that the matrices used in this paper are denoted differently to those in cited literature.

Theorem 1 ([2], Thm. 2.14) *Let $A = BD \in \mathbb{R}^{m \times n}$, $m \geq n$, where B has unit columns and D is diagonal, be of full column rank. Let δA be such that $\|\delta A D^{-1}\|_2 < \sigma_{\min}(B)$. Then*

$$\frac{|\sigma_i(A) - \sigma_i(A + \delta A)|}{\sigma_i(A)} \leq \frac{\|\delta A D^{-1}\|_2}{\sigma_{\min}(B)}. \quad (1)$$

Hence, if B is well-conditioned with $\sigma_{\min}(B) \approx O(1)$ and the *scaled* perturbation $\delta A D^{-1}$ is small in 2-norm, *all* singular values will ‘feel’ a relatively tiny change. Note that the diagonal elements of D can be huge. Also note that the perturbed matrix can be written as: $A + \delta A = (B + \delta A D^{-1})D$. The condition $\|\delta A D^{-1}\|_2 < \sigma_{\min}(B)$ warrants that the perturbed matrix $A + \delta A$ remains of full column rank.

The next theorem provides the upper bound for the scaled forward error in the matrix-matrix multiplication $fl(VA)$ when V is exactly orthogonal.

Theorem 2 ([5], Thm. 3.1) *Let $V \in \mathbb{R}^{m \times m}$ be orthogonal and let $A = BD \in \mathbb{R}^{m \times n}$, $m \geq n$, be as in Theorem 1. Then in finite precision arithmetic with precision $\mathbf{u}$*

$$\|[VA - fl(VA)]D^{-1}\|_2 \leq c\sqrt{n}\mathbf{u}, \quad (2)$$

where $c = 2(m-1)\sqrt{m}$. If V is an elementary orthogonal matrix then (2) holds with $c = 2\sqrt{2} \leq 3$, and if Q is a Householder reflection (applied as $A_1 = A - v(Av)^T$) then (2) holds with $c = 4m$.

In Theorem 1, one works with the scaled *additive* perturbation of A . The next theorem uses the *multiplicative* perturbation(s).

Theorem 3 ([3], Thm. 2.2) *Suppose $\tilde{A} = (I + E)A(I + F)$, with $\|E\|_2 = \eta_E$ and $\|F\|_2 = \eta_F$. Let $\eta = \max(\eta_E, \eta_F)$ and $\eta' = 2\eta + \eta^2$. Then*

$$\frac{|\sigma_i(A) - \sigma_i(\tilde{A})|}{\sigma_i(A)} \leq \eta_E + \eta_F + \eta_E\eta_F \leq \eta'. \quad (3)$$

Of course, to warrant small relative changes in *all* singular values, the value of η' has to be of order $O(\mathbf{u})$.

Finally, we need some information about changes of left and right singular vectors under perturbation. In the following, the i th singular triplet of A and $\tilde{A}$ is denoted by $(u_i, \sigma_i(A), v_i)$ and $(\tilde{u}_i, \sigma_i(\tilde{A}), \tilde{v}_i)$, respectively.

Theorem 4 ([3], Thm. 2.3) *Suppose $\tilde{A} = (I + E)A(I + F)$, with $\|E\|_2 = \eta_E$ and $\|F\|_2 = \eta_F$. Let $\eta = \max(\eta_E, \eta_F)$ and $\eta' = 2\eta + \eta^2$. Then the acute angle θ between u_i and $\tilde{u}_i$ (or between v_i and $\tilde{v}_i$) is bounded by*

$$\sin \theta \leq \sqrt{2} \left(\frac{1 + \eta'}{1 - \eta'} \cdot \frac{\eta'}{\text{relgap}(i, A) - \eta'} + \eta \right) \quad (4)$$

provided that the relative gap

$$\text{relgap}(i, A) \equiv \min \left(\min_{j \neq i} \frac{|\sigma_i(A) - \sigma_j(\tilde{A})|}{\sigma_i(A)}, 2 \right) \quad (5)$$

between $\sigma_i(A)$ and the nearest other singular value of $\tilde{A}$ is larger than η' , i.e. $\text{relgap}(i, A) > \eta'$.

As noted in [3], there are various variants of this theorem which use a different definition of the relative gap. Note that in Theorem 4 the relative gap $\text{relgap}(i, A)$ is defined using the singular values of *two different* matrices. At first sight, $\sin \theta$ is small when all η_E and η_F and η' are tiny and $\text{relgap}(i, A)$ is relatively large (i.e., $\sigma_i(A)$ is well separated from other singular values of $\tilde{A}$). Hence, in the case of a tight cluster of singular values, it is much better to work with the whole singular subspace corresponding to that cluster than with individual singular vectors.

3 Perturbation Analysis

3.1 Computing $\text{fl}(VA)$, V exactly orthogonal

We start with the case when V is exactly orthogonal and all matrices are real, square and non-singular of order n . Recall that $A = BD$, where B is well-conditioned with unit columns and D is diagonal. Define $C \equiv VA$ and $\hat{C}' \equiv \text{fl}(VA)$. Then, according to Theorem 2, the column-scaled forward error $\delta C D^{-1} = (\hat{C}' - C)D^{-1}$ has the upper bound :

$$\|\delta C D^{-1}\|_2 \leq c\sqrt{n}\mathbf{u}.$$

Let us assume that $c\sqrt{n}\mathbf{u} < \sigma_{\min}(B)$, i.e. $\sigma_{\min}(B)$ is not too small. This assumption is reasonable for a well-conditioned B . Then according to Theorem 1:

$$\frac{|\sigma_i(\hat{C}') - \sigma_i(C)|}{\sigma_i(C)} \leq c\sqrt{n} \sigma_{\min}(B)^{-1} \mathbf{u}, \quad 1 \leq i \leq n. \quad (6)$$

Since B has unit columns, $\sigma_{\max}(B) \geq 1$ and the upper bound in (6) can be written as $c\sqrt{n}\kappa_2(B)\mathbf{u}$. Moreover, since V is exactly orthogonal, the matrices $C = VA$ and A have the same singular values. Consequently, $\sigma_i(C) = \sigma_i(A)$ and (6) gives the upper bound for the relative change of singular values of A . Hence, the multiplication of A by an exactly orthogonal V using the floating point arithmetic causes only small relative errors in *all* singular values of a column-graded A .

3.2 Computing $\mathcal{H}(\hat{V}A)$, $\hat{V}$ numerically orthogonal

Now assume that we compute $\hat{C} \equiv \mathcal{H}(\hat{V}A)$, where $A \in \mathbb{R}^{m \times n}$, $m \geq n$, and $\hat{V}$ is numerically orthogonal of order m , i.e., there exist an exactly orthogonal V and perturbation δV such that

$$\hat{V} = V + \delta V, \quad \|\delta V\|_2 = \epsilon_1 \approx O(\mathbf{u}). \quad (7)$$

Such a situation arises, for example, if $\hat{V}$ is the product of Householder reflections and/or Givens rotations in floating point arithmetic. This is exactly the case of our application where $\hat{V}$ is the matrix of eigenvectors of the symmetric factor in the polar decomposition of A^T computed by the Divide-and-Conquer algorithm (DCA).

In the following, we derive the upper bound for the relative change of all singular values between matrices $A = BD$ and $\hat{C} = \mathcal{H}(\hat{V}A)$. As is well known (see [4, p. 71]),

$$|\mathcal{H}(\hat{V}A) - \hat{V}A| \leq \gamma_m |\hat{V}| |A|,$$

where $\gamma_m = m\mathbf{u}/(1 - m\mathbf{u})$ for $m\mathbf{u} < 1$ and the matrix inequalities involving the absolute value are understood element-wise. Then

$$|\mathcal{H}(\hat{V}A) - \hat{V}A| D^{-1} \leq \gamma_m |\hat{V}| |A| D^{-1},$$

since D^{-1} is diagonal with positive diagonal elements. But the last relationship between matrices is equivalent to

$$|[\mathcal{H}(\hat{V}A) - \hat{V}A] D^{-1}| \leq \gamma_m |\hat{V}| |B|,$$

where $B = AD^{-1}$ is well-conditioned. Hence, using the 2-norm and the Frobenius norm, one gets

$$\begin{aligned} \|[\mathcal{H}(\hat{V}A) - \hat{V}A] D^{-1}\|_2 &\leq \|[\mathcal{H}(\hat{V}A) - \hat{V}A] D^{-1}\|_F \leq \gamma_m \|\hat{V}\|_F \|B\|_F \\ &\leq \gamma_m \|\hat{V}\|_F \|B\|_F = \gamma_m \|\hat{V}\|_F \|B\|_F \\ &\leq \gamma_m (\|V\|_F + \|\delta V\|_F) \|B\|_F \leq \gamma_m (\sqrt{m} + \sqrt{m}\epsilon_1) \sqrt{n}. \end{aligned}$$

Finally, assuming $m\mathbf{u} \leq 0.5$, the upper bound reads

$$\|[\mathcal{H}(\hat{V}A) - \hat{V}A] D^{-1}\|_2 \leq 2m\sqrt{m}(1 + \epsilon_1)\sqrt{n}\mathbf{u} \approx 2m\sqrt{m}\sqrt{n}\mathbf{u}, \quad (8)$$

because $\epsilon_1\mathbf{u} \approx O(\mathbf{u}^2)$ and can be omitted. Note that (8) is the extension of (2), which is valid for an exactly orthogonal V , to the case when $\hat{V}$ is only numerically orthogonal.

However, we can not use (6) as the upper bound for the relative change of $\sigma_i(A)$, because $\sigma_i(A) \neq \sigma_i(\hat{V}A)$, $1 \leq i \leq n$ (since $\hat{V}$ is not exactly orthogonal). Therefore, we derive the relationship between matrices $\hat{C}$ and A in the form of a *multiplicative* perturbation of A .

Let $C \equiv \hat{V}A = \hat{V}BD$, $\delta C \equiv \hat{C} - C$, and let us write:

$$\begin{aligned}\hat{C} &= fl(\hat{V}A) = \hat{V}BD + \delta C = (V + \delta V)BD + \delta C \\ &= VBD + \delta VBD + \delta C = V(I + V^T\delta V + V^T\delta C D^{-1}B^+)BD \\ &= V(I + X + Y)A, \quad \text{where } X \equiv V^T\delta V, Y \equiv V^T\delta C D^{-1}B^+, \end{aligned}$$

where B^+ denotes the Moore-Penrose pseudoinverse of B . Note that $\|X\|_2 = \|\delta V\|_2$. Moreover, $\delta C = fl(\hat{V}A) - \hat{V}A$, and from (8) one gets

$$\|Y\|_2 = \|V^T\delta C D^{-1}B^+\|_2 \leq 2m\sqrt{m}\sqrt{n}\sigma_{\min}(B)^{-1}\mathbf{u}.$$

Finally, using $E \equiv X + Y$, one has $\hat{C} = V(I + E)A$. Now apply Theorems 3 and 4 to the matrices A and $\tilde{A} \equiv (I + E)A$ with

$$\eta_E = \|E\|_2 \leq 2m\sqrt{m}\sqrt{n}\sigma_{\min}(B)^{-1}\mathbf{u} + \|\delta V\|_2 \leq 2m\sqrt{m}\sqrt{n}\kappa_2(B)\mathbf{u} + \|\delta V\|_2 \quad (9)$$

and $\eta_F = 0$, so that $\eta = \eta_E$ and $\eta' = 2\eta_E + \eta_E^2$. Since η_E^2 is of order $O(\kappa_2^2(B)\mathbf{u}^2)$, it can be omitted for a well-conditioned B .

However, Theorems 3 and 4 describe the relationship between the corresponding singular triplets of A and $\tilde{A}$ and *not* between A and $\hat{C}$. But note that $\hat{C} = V\tilde{A}$ where V is exactly orthogonal.

Let $A = P\Sigma S^T$, $\tilde{A} = \tilde{P}\tilde{\Sigma}\tilde{S}^T$ and $\hat{C} = \hat{U}\hat{\Sigma}\hat{W}^T$ be the corresponding thin SVDs of matrices A , $\tilde{A}$ and $\hat{C}$, respectively. Since V is exactly orthogonal, $\hat{C} = V\tilde{A} = (V\tilde{P})\tilde{\Sigma}\tilde{S}^T$ is the SVD of $\hat{C}$, so that $\hat{U} = V\tilde{P}$, $\hat{\Sigma} = \tilde{\Sigma}$ and $\hat{W} = \tilde{S}$. We are interested in the relative difference between singular triplets of $\hat{C}$ and A , i.e., between $(\hat{u}_i, \sigma_i(\hat{C}), \hat{w}_i)$ and $(p_i, \sigma_i(A), s_i)$. Note that Theorems 3 and 4 bound the relative changes between singular triplets of matrices $\tilde{A}$ (not $\hat{C}$) and A , i.e., the bounds are valid for the angles $\angle(\tilde{p}_i, p_i)$, $\angle(\tilde{s}_i, s_i)$, and for the singular values $\sigma_i(\tilde{A})$ and $\sigma_i(A)$. Fortunately, $\sigma_i(\hat{C}) = \sigma_i(\tilde{A})$ and $\hat{w}_i = \tilde{s}_i$, so we have bounds between corresponding singular values of $\hat{C}$ and A and between corresponding right singular vectors of $\hat{C}$ and A . But we have *no bound* for the angle $\angle(\hat{u}_i, p_i)$, because the orthogonal transformation $\hat{u}_i = V\tilde{p}_i$ can change the direction of $\tilde{p}_i$ by any angle. Consequently, also the angle $\angle(\hat{u}_i, p_i)$ can be of any value.

However, having the computed vector $\hat{u}_i$ and the numerically orthogonal $\hat{V}$, one can try to *recover* the corresponding left singular vector p_i of A using the vector $\hat{p}_i \equiv fl(\hat{V}^T\hat{u}_i)$, which is computed in the floating point arithmetic. Also note the relationship between the left singular vectors of $\hat{C}$ and $\tilde{A}$: $\tilde{p}_i = V^T\hat{u}_i$, where V is exactly orthogonal.

For any two vectors x and y of unit length, the acute angle $\theta \in [0, \pi/2]$ between them is related to the $\|x - y\|_2$ by

$$\|x - y\|_2^2 = \|x\|_2^2 - 2x^Ty + \|y\|_2^2 = 2 - 2\cos\theta = 4\sin^2(\theta/2),$$

so that $\|x - y\|_2 = 2\sin(\theta/2)$, since the sine is non-negative in the interval $[0, \pi/2]$. Hence,

$$\sin\theta = 2\sin(\theta/2)\cos(\theta/2) \leq 2\sin(\theta/2) = \|x - y\|_2.$$

Next we bound $\|\hat{p}_i - p_i\|_2$ from above in several steps. Here we assume that all singular vectors in the SVD of A , $\tilde{A}$ and $\hat{C}$ are of unit Euclidean norm. However, $\hat{p}_i = fl(\hat{V}^T \hat{u}_i)$ is not normalized.

Let us write:

$$\begin{aligned} \|\hat{p}_i - p_i\|_2 &= \|fl(\hat{V}^T \hat{u}_i) - p_i\|_2 \leq \|fl(\hat{V}^T \hat{u}_i) - \hat{V}^T \hat{u}_i\|_2 + \|\hat{V}^T \hat{u}_i - V^T \hat{u}_i\|_2 + \\ &\quad + \|V^T \hat{u}_i - \tilde{p}_i\|_2 + \|\tilde{p}_i - p_i\|_2. \end{aligned}$$

By definition, $\|V^T \hat{u}_i - \tilde{p}_i\|_2 = 0$. From (8) with $n = 1$ and $d_{11} = 1$ one gets $\|fl(\hat{V}^T \hat{u}_i) - \hat{V}^T \hat{u}_i\|_2 \leq 2m\sqrt{m}\mathbf{u}$, and the next term is bounded by $\|\hat{V}^T \hat{u}_i - V^T \hat{u}_i\|_2 \leq \|\delta V\|_2$. Regarding the last term, $\|\tilde{p}_i - p_i\|_2$, we use Theorem 4 for the matrix pair $(A, \tilde{A})$ and the fact that the sine is an increasing function on the interval $[0, \pi/2]$:

$$\begin{aligned} \|\tilde{p}_i - p_i\|_2 &= 2 \sin(\angle(\tilde{p}_i, p_i)/2) \leq 2 \sin \angle(\tilde{p}_i, p_i) \\ &\leq 2\sqrt{2} \left(\frac{1 + \eta'}{1 - \eta'} \cdot \frac{\eta'}{\text{relgap}(i, A) - \eta'} + \eta_E \right), \end{aligned}$$

where η_E is bounded in (9) and $\eta' = 2\eta_E + \eta_E^2$. Finally, the sum of three previous upper bounds provides the result:

$$\|\hat{p}_i - p_i\|_2 \leq 2m\sqrt{m}\mathbf{u} + \|\delta V\|_2 + 2\sqrt{2} \left(\frac{1 + \eta'}{1 - \eta'} \cdot \frac{\eta'}{\text{relgap}(i, A) - \eta'} + \eta_E \right). \quad (10)$$

Recall that $A = BD$, $\|\delta V\|_2 \approx O(\mathbf{u})$ and $\eta_E \approx O(\kappa_2(B)\mathbf{u})$. Hence, for a well-conditioned B and a well separated singular value σ_i of A with its relatively large relative gap, one has $\|\hat{p}_i - p_i\|_2 \approx O(\mathbf{u})$, which implies two facts: 1) $|\|\hat{p}_i\|_2 - 1| \approx O(\mathbf{u})$ (since $\|p_i\|_2 = 1$), and 2) $\sin \angle(\hat{p}_i, p_i) \approx O(\mathbf{u})$. Consequently, the computed vector $\hat{p}_i = fl(\hat{V}^T \hat{u}_i)$ can be considered as a good approximation of the left singular vector p_i of A .

Alternatively, we can directly compute $\|\hat{p}_i\|_2$ in floating point arithmetic and bound the term $|fl(\|\hat{p}_i\|_2) - 1|$ (or $fl(\|\hat{p}_i\|_2)$) from both sides. It will be shown that $|fl(\|\hat{p}_i\|_2) - 1| \approx O(\mathbf{u})$.

We start with the computation of $\hat{p}_i = fl(\hat{V}^T \hat{u}_i)$. Using the backward error result for a matrix-vector multiplication (see [4, p. 69]), this can be written as

$$\hat{p}_i = (\hat{V}^T + \delta \hat{V}^T) \hat{u}_i = (V^T + \delta V^T + \delta \hat{V}^T) \hat{u}_i \quad \text{with} \quad |\delta \hat{V}^T| \leq \gamma_m |\hat{V}^T|,$$

so that

$$\|\delta \hat{V}\|_2 \leq \|\delta \hat{V}\|_F \leq \gamma_m \|\hat{V}\|_F \leq \gamma_m \sqrt{m} \|\hat{V}\|_2 \leq \gamma_m \sqrt{m} (\|V\|_2 + \|\delta V\|_2) \approx \gamma_m \sqrt{m},$$

because $\gamma_m \sqrt{m} \|\delta V\|_2 \approx O(\mathbf{u}^2)$ and can be omitted.

Next, let us compute $fl(\|\hat{p}_i\|_2^2) = fl(\hat{p}_i^T \hat{p}_i)$. Using the floating point analysis of computing a scalar product of two vectors (see [4, p. 63]), one has

$$|fl(\hat{p}_i^T \hat{p}_i) - \hat{p}_i^T \hat{p}_i| \leq \gamma_m |\hat{p}_i^T| |\hat{p}_i|. \quad (11)$$

Now we bound, under reasonable assumption, the term $\hat{p}_i^T \hat{p}_i$ on the left-hand side of (11) from both sides. The upper bound is as follows:

$$\begin{aligned} 0 < \hat{p}_i^T \hat{p}_i &= |\hat{u}_i^T (V + \delta V + \delta \hat{V}) (V^T + \delta V^T + \delta \hat{V}^T) \hat{u}_i| \\ &\leq 1 + |\hat{u}_i^T \delta V V^T \hat{u}_i| + |\hat{u}_i^T \delta \hat{V} V^T \hat{u}_i| + |\hat{u}_i^T V \delta V^T \hat{u}_i| + |\hat{u}_i^T \delta V \delta V^T \hat{u}_i| + \\ &\quad + |\hat{u}_i^T \delta \hat{V} \delta V^T \hat{u}_i| + |\hat{u}_i^T V \delta \hat{V}^T \hat{u}_i| + |\hat{u}_i^T \delta V \delta \hat{V}^T \hat{u}_i| + |\hat{u}_i^T \delta \hat{V} \delta V^T \hat{u}_i|. \end{aligned}$$

Each of 8 terms above represents the absolute value of a scalar product of two vectors, which can be bounded from above using the Cauchy-Schwartz inequality. Each scalar product contains two matrices and the upper bound will contain the product of 2-norms of those matrices. However, each matrix with the prefix ‘ δ ’ has its 2-norms of order $O(\mathbf{u})$, so that their product is of order $O(\mathbf{u}^2)$ and will be omitted. Consequently, up to the first order of $\mathbf{u}$,

$$\begin{aligned} \hat{p}_i^T \hat{p}_i &\leq 1 + |\hat{u}_i^T \delta V V^T \hat{u}_i| + |\hat{u}_i^T \delta \hat{V} V^T \hat{u}_i| + |\hat{u}_i^T V \delta V^T \hat{u}_i| + |\hat{u}_i^T V \delta \hat{V}^T \hat{u}_i| \\ &\leq 1 + \|\delta V^T \hat{u}_i\|_2 \|V^T \hat{u}_i\|_2 + \|\delta \hat{V}^T \hat{u}_i\|_2 \|V^T \hat{u}_i\|_2 + \|V^T \hat{u}_i\|_2 \|\delta V^T \hat{u}_i\|_2 + \\ &\quad + \|V^T \hat{u}_i\|_2 \|\delta \hat{V}^T \hat{u}_i\|_2 \\ &\leq 1 + 2(\|\delta V\|_F + \|\delta \hat{V}\|_F) \leq 1 + 2\sqrt{m}(\|\delta V\|_2 + \|\delta \hat{V}\|_2) \\ &\leq 1 + 2\sqrt{m} \|\delta V\|_2 + 2m\gamma_m, \end{aligned} \tag{12}$$

since $\|\hat{u}_i\|_2 = \|V^T \hat{u}_i\|_2 = 1$.

We can also bound $\hat{p}_i^T \hat{p}_i$ from below. However, to be of any use, one assumption will be needed. To this end, taking the terms up to $O(\mathbf{u})$,

$$\begin{aligned} \hat{p}_i^T \hat{p}_i &\geq 1 - |\hat{u}_i^T \delta V V^T \hat{u}_i| - |\hat{u}_i^T \delta \hat{V} V^T \hat{u}_i| - |\hat{u}_i^T V \delta V^T \hat{u}_i| - |\hat{u}_i^T V \delta \hat{V}^T \hat{u}_i| \\ &\geq 1 - 2(\|\delta V\|_F + \|\delta \hat{V}\|_F) \geq 1 - 2\sqrt{m}(\|\delta V\|_2 + \|\delta \hat{V}\|_2) \\ &\geq 1 - (2\sqrt{m} \|\delta V\|_2 + 2m\gamma_m), \end{aligned} \tag{13}$$

where we assume that $2\sqrt{m} \|\delta V\|_2 + 2m\gamma_m < 1$, so that the final lower bound remains positive.

Finally, the upper bound of the right-hand side of (11) up to the first order of $\mathbf{u}$ can be derived as follows:

$$\begin{aligned} \gamma_m |\hat{p}_i^T| |\hat{p}_i| &= \gamma_m \|\hat{p}_i\|_2^2 = \gamma_m \|(V^T + \delta V^T + \delta \hat{V}^T) \hat{u}_i\|_2^2 \\ &\leq \gamma_m [(\|V\|_2 + \|\delta V\|_2 + \|\delta \hat{V}\|_2) \|\hat{u}_i\|_2]^2 \\ &= \gamma_m (1 + \|\delta V\|_2 + \|\delta \hat{V}\|_2)^2 \approx \gamma_m, \end{aligned} \tag{14}$$

since γ_m itself is of order $O(\mathbf{u})$. It follows from (11) that

$$\hat{p}_i^T \hat{p}_i - \gamma_m |\hat{p}_i^T| |\hat{p}_i| \leq \mathcal{f}(\|\hat{p}_i\|_2^2) \leq \hat{p}_i^T \hat{p}_i + \gamma_m |\hat{p}_i^T| |\hat{p}_i|.$$

Using (12), (13) and (14), one gets

$$1 - [2\sqrt{m} \|\delta V\|_2 + (2m + 1)\gamma_m] \leq \mathcal{f}(\|\hat{p}_i\|_2^2) \leq 1 + [2\sqrt{m} \|\delta V\|_2 + (2m + 1)\gamma_m].$$

Assuming additionally that $\zeta \equiv 2\sqrt{m}\|\delta V\|_2 + (2m+1)\gamma_m \ll 1$, the final bounds for $\text{fl}(\|\hat{p}_i\|_2)$ read

$$1 - \zeta/2 \leq \text{fl}(\|\hat{p}_i\|_2) \leq 1 + \zeta/2, \quad \zeta \approx O(\mathbf{u}), \quad (15)$$

where the rounding error coming from the computation of one square root was omitted. Recall that the corresponding left singular p_i of A has $\|p_i\|_2 = 1$ exactly. The bounds in (15) show that $|\text{fl}(\|\hat{p}_i\|_2) - 1| \approx O(\mathbf{u})$, i.e., the Euclidean norms of $\hat{p}_i = \text{fl}(\hat{V}^T \hat{u}_i)$ and p_i are equal up to $O(\mathbf{u})$. Consequently, it follows from (10) that $\angle(\hat{p}_i, p_i) \approx O(\mathbf{u})$ for a well separated singular value $\sigma_i(A)$.

The results of the above analysis are summarized in the next theorem.

Theorem 5 *Let $A = BD \in \mathbb{R}^{m \times n}$, $m \geq n$, where $B \in \mathbb{R}^{m \times n}$ is well-conditioned with columns of unit Euclidean norm and D is diagonal of order n . Let $\hat{V} \in \mathbb{R}^{m \times m}$ be numerically orthogonal, i.e., an $O(\mathbf{u})$ perturbation of some exactly orthogonal matrix V w.r.t. the 2-norm. Finally, let $\hat{C} = \text{fl}(\hat{V}A)$. Then for all indices i , $1 \leq i \leq n$:*

1. *The relative error between corresponding singular values $\sigma_i(\hat{C})$ and $\sigma_i(A)$ is of order $O(\kappa_2(B)\mathbf{u})$.*
2. *The sine of an acute angle between corresponding right singular vectors $\hat{w}_i$ and s_i of matrices $\hat{C}$ and A , respectively, is of order $O(\kappa_2(B)\mathbf{u})$ for a well separated singular value $\sigma_i(A)$.*
3. *The left singular vector p_i of A that corresponds to the left singular vector $\hat{u}_i$ of $\hat{C}$ can be recovered by computing $\hat{p}_i = \text{fl}(\hat{V}^T \hat{u}_i)$ with $|\text{fl}(\|\hat{p}_i\|_2) - 1| \approx O(\mathbf{u})$ and $\angle(\hat{p}_i, p_i) \approx O(\mathbf{u})$ for a well separated singular value $\sigma_i(A)$.*

4 Loss of Orthogonality in Computing $C = A\hat{V}$, $\hat{V}$ Numerically Orthogonal

In our application described in [1], we precondition a matrix A by a numerically orthogonal matrix $\hat{V}$, which is the eigenvector matrix of the Hermitian factor H and comes from the (partial) PD of A . If $A = P\Sigma S^T$ is the thin SVD of $A \in \mathbb{R}^{m \times n}$, $m \geq n$, then in exact arithmetic the exactly orthogonal V of order n will be the matrix of right singular vectors of A , $V = S$, and $AV = U\Sigma$. However, in our case $\hat{V} = V + \delta V$ for some orthogonal V and, moreover, $V \neq S$, if we approximate H by performing only a given number of Halley's iterations. Hence, the orthogonal V is a perturbation of S , i.e., $V = S + \delta S$. Consequently,

$$\hat{V} = S + \delta S + \delta V, \quad S \text{ and } (S + \delta S) \text{ orthogonal,}$$

where $\|\delta V\|_2 \approx O(\mathbf{u})$, while $\|\delta S\|_2$ will depend, e.g., on the used number of Halley's iterations. Hence, while $\|\delta V\|_2$ is tiny, $\|\delta S\|_2$ may be large.

Numerical results from [1] show, that the computed $\hat{C} = \text{fl}(A\hat{V})$ shows a substantial loss of the orthogonality of its columns when A is ill-conditioned. The aim of this section is to qualitatively understand this loss of orthogonality.

To get some insight, we provide the analysis in *exact* arithmetic. Write

$$C = A\hat{V} = AS + A\delta S + A\delta V = P\Sigma + A\delta S + A\delta V.$$

The loss of orthogonality in columns of C will be measured by

$$\omega \equiv \|(C\Sigma^{-1})^T(C\Sigma^{-1}) - I\|_2 = \|\Sigma^{-1}CC^T\Sigma^{-1} - I\|_2. \quad (16)$$

Note that if $\hat{V} = S$ (i.e., $\delta S = \delta V = 0$), then $A\hat{V} = P\Sigma$, $\Sigma^{-1}C^TC\Sigma^{-1} = I$, $\omega = 0$ and we are done—there is no need of the subsequent Jacobi algorithm applied to AS .

Let us compute C^TC :

$$\begin{aligned} C^TC &= (\Sigma P^T + \delta S^T A^T + \delta V^T A^T) \cdot (P\Sigma + A\delta S + A\delta V) \\ &= \Sigma^2 + \delta S^T A^T P\Sigma + \delta V^T A^T P\Sigma + \Sigma P^T A\delta S + \delta S^T A^T A\delta S + \\ &\quad + \delta V^T A^T A\delta S + \Sigma P^T A\delta V + \delta S^T A^T A\delta V + \delta V^T A^T A\delta V \\ &= \Sigma^2 + \delta S^T S\Sigma^2 + \delta V^T S\Sigma^2 + \Sigma^2 S^T \delta S + \delta S^T S\Sigma^2 S^T \delta S + \\ &\quad + \delta V^T S\Sigma^2 S^T \delta S + \Sigma^2 S^T \delta V + \delta S^T S\Sigma^2 S^T \delta V + \delta V^T S\Sigma^2 S^T \delta V, \end{aligned}$$

where we used $A^T A = S\Sigma^2 S^T$ and $A^T P = S\Sigma$. Then:

$$\begin{aligned} \Sigma^{-1}C^TC\Sigma^{-1} - I &= \Sigma^{-1}\delta S^T S\Sigma + \Sigma^{-1}\delta V^T S\Sigma + \Sigma S^T \delta S\Sigma^{-1} + \\ &\quad + \Sigma^{-1}\delta S^T S\Sigma^2 S^T \delta S\Sigma^{-1} + \Sigma^{-1}\delta V^T S\Sigma^2 S^T \delta S\Sigma^{-1} + \Sigma S^T \delta V\Sigma^{-1} + \\ &\quad + \Sigma^{-1}\delta S^T S\Sigma^2 S^T \delta V\Sigma^{-1} + \Sigma^{-1}\delta V^T S\Sigma^2 S^T \delta V\Sigma^{-1}. \end{aligned}$$

Next, we bound the 2-norm of each of 8 terms above:

$$\begin{aligned} \|\Sigma^{-1}\delta S^T S\Sigma\|_2 &\leq \kappa_2(A) \|\delta S\|_2, \quad \|\Sigma^{-1}\delta V^T S\Sigma\|_2 \leq \kappa_2(A) \|\delta V\|_2, \\ \|\Sigma S^T \delta S\Sigma^{-1}\|_2 &\leq \kappa_2(A) \|\delta S\|_2, \quad \|\Sigma^{-1}\delta S^T S\Sigma^2 S^T \delta S\Sigma^{-1}\|_2 \leq \kappa_2^2(A) \|\delta S\|_2^2, \\ \|\Sigma^{-1}\delta V^T S\Sigma^2 S^T \delta S\Sigma^{-1}\|_2 &\leq \kappa_2^2(A) \|\delta S\|_2 \|\delta V\|_2, \\ \|\Sigma S^T \delta V\Sigma^{-1}\|_2 &\leq \kappa_2(A) \|\delta V\|_2, \\ \|\Sigma^{-1}\delta S^T S\Sigma^2 S^T \delta V\Sigma^{-1}\|_2 &\leq \kappa_2^2(A) \|\delta S\|_2 \|\delta V\|_2, \\ \|\Sigma^{-1}\delta V^T S\Sigma^2 S^T \delta V\Sigma^{-1}\|_2 &\leq \kappa_2^2(A) \|\delta V\|_2^2. \end{aligned}$$

Hence, the final bound for the loss of orthogonality of columns in matrix C has the form:

$$\begin{aligned} \omega = \|\Sigma^{-1}C^TC\Sigma^{-1} - I\|_2 &\leq 2\kappa_2(A) (\|\delta S\|_2 + \|\delta V\|_2) + 2\kappa_2^2(A) \|\delta S\|_2 \|\delta V\|_2 + \\ &\quad + \kappa_2^2(A) (\|\delta S\|_2^2 + \|\delta V\|_2^2). \end{aligned} \quad (17)$$

According to the above analysis, the main factor in the loss of orthogonality of columns in $C = A\hat{V}$ is the difference δS between $V = \hat{V} - \delta V$ and S , where S is the matrix of right singular vectors of A . In the case of (very) ill-conditioned A , the difference δS may be amplified by $\kappa_2(A)$, and this amplification can

lead to a substantial loss of orthogonality of columns in C . If $\|\delta S\|_2 \ll 1$ and $\kappa_2(A)$ is not too large, then the last two terms in the sum on the right-hand side of (17) containing $\kappa_2^2(A)$ can be omitted. However, for very large values of $\kappa_2(A)$ (say, $\kappa_2(A) \geq 1/\sqrt{\mathbf{u}}$) and not-so-small $\|\delta S\|_2$, the term $\kappa_2^2(A) \|\delta S\|_2^2$ can also contribute to some extent. We have observed such a substantial loss of orthogonality in [1, Table 2] where for $\kappa_2(A) = 10^{10}$ and using only one Halley's iteration for the PD of A , the OSBJA with dynamic ordering started with the approximate maximal weight $maxw \approx 5.4 \times 10^{-4}$, whereas for a well-conditioned matrix with $\kappa_2(A) = 10^2$ this value was $maxw \approx 7.0 \times 10^{-13}$ (see [1, Table 1])—a difference of about 9 orders of magnitude! It is interesting to note that the ratio of the 2-norm condition numbers of corresponding matrices was 10^8 , i.e., 8 orders of magnitude, which is in agreement with the upper bound (17).

On the other hand, even if $\|\delta S\|_2 = 0$, i.e., even if the Halley's iterations converged fully and provided an exact S , the loss of orthogonality ω would have the non-vanishing upper bound

$$\omega \leq 2\kappa_2(A) \|\delta V\|_2 + \kappa_2^2(A) \|\delta V\|_2^2, \quad \|\delta V\|_2 \approx O(\mathbf{u}).$$

For $\kappa_2(A) = 10^{10}$, $\mathbf{u} \approx 1.1 \times 10^{-16}$ and omitting the term of order $O(\mathbf{u}^2)$, one gets $\omega \leq 2.2 \times 10^{-6}$, which is in agreement with the numerical experiment in [1, Table 2] using 6 Halley's iterations (similarly for $\kappa_2(A) = 10^2$ in [1, Table 1] using 5 Halley's iterations).

In the next section, the loss of orthogonality of columns of C is illustrated by numerical experiments using random matrices with an arithmetic or geometric sequence of singular values and the 2-norm condition number ranging from 10^1 to 10^8 .

5 Numerical Experiments

All numerical experiments were performed in MATLAB using double precision with the round-off unit $\mathbf{u} \approx 1.11 \times 10^{-16}$. For each condition number $\kappa_2 \in \{10^1, 10^2, 10^4, 10^6, 10^8\}$, 100 random, $N(0, 1)$ -distributed matrices of dimensions $m \times n = 700 \times 200$ were generated as follows. First, an orthogonal matrix S of order n was computed from the QR decomposition of a $N(0, 1)$ -distributed random matrix X of order n , and the Hermitian factor H was computed as $H = SAS^T$, where A was a diagonal matrix of order n with the eigenvalues of H distributed in the interval $[\kappa_2^{-1}(A), 1]$ as the arithmetic ($\lambda_i = 1 - (i-1)(1 - \kappa_2^{-1}(A))/(n-1)$, $1 \leq i \leq n$), or geometric sequence ($\lambda_i = \kappa_2(A)^{-(i-1)/(n-1)}$). Note that both sequences were constructed in descending order. Second, another orthogonal matrix U of order m was computed from the QR decomposition of a $N(0, 1)$ -distributed random matrix Y of order m , and its first n columns were used for the construction of the test matrix $A = U(:, 1:n)H$ given in the form of its PD. Hence, the matrix S was also the matrix of right singular vectors of A and $\lambda_i(H) = \sigma_i(A)$, where $\sigma_i(A)$ is the i th largest singular value (SV) of A .

Each matrix A then entered the subroutine for its *computed* (approximate) PD using k Halley's iterations (see [1]), which delivers the Hermitian factor $\hat{H}$. Afterwards, the EVD of $\hat{H} = V\hat{\Lambda}V^T$ was computed using the MATLAB function `eig()`. Here we omit the symbol 'hat' over the computed matrix V . In our experiments, the value of k was either $k = 1$ (only the beginning of convergence) or $k = 6$ (full convergence of Halley's iterations). In all figures below, a matrix A is identified by a global matrix index (GMI); its relation to $\kappa_2(A)$ is given in Table 1.

Table 1. Global matrix index vs. $\kappa_2(A)$

	$\kappa_2(A)$				
	10^1	10^2	10^4	10^6	10^8
index	1–100	101–200	201–300	301–400	401–500

Results of numerical experiments for the arithmetically distributed SVs are depicted in Fig. 1 and Fig. 2 for $k = 1$ and $k = 6$, respectively.

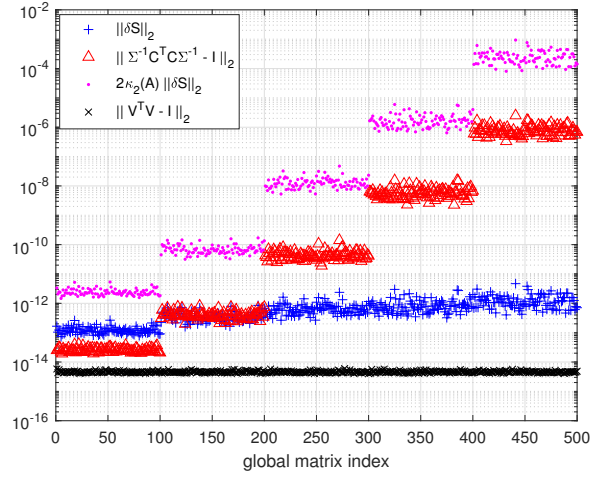


Fig. 1. Results using 1 Halley's iteration and an arithmetic sequence of SVs

In general, the values of $\|\delta S\|_2 = \|V - S\|_2$ and $\omega = \|\Sigma^{-1}C^T C \Sigma^{-1} - I\|_2$ (where $C = AV$) show quite a large dispersion for $k = 1$ Halley's iteration (HI) and are more stabilized for $k = 6$ HI. The numerical orthogonality of the computed V is on the level $\approx 8 \times 10^{-15}$ regardless to k , so that we can work

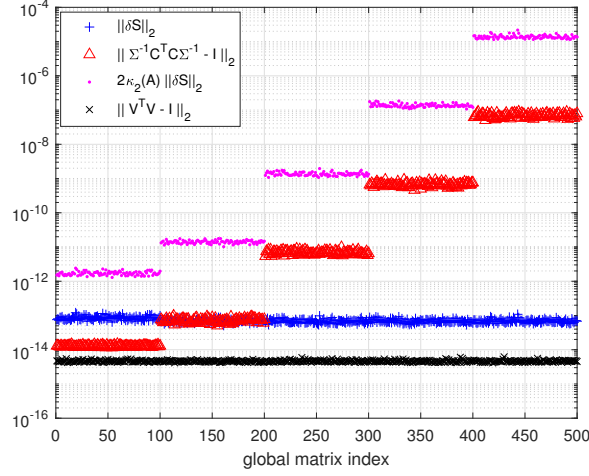


Fig. 2. Results using 6 Halley's iterations and an arithmetic sequence of SVs

with the assumption of $\|\delta V\|_2 \approx 0$. As expected, in both cases the value of $\|\delta S\|_2$ does not depend on $\kappa_2(A)$, since the quality of the computed polar decomposition using Halley's iterations should not depend on $\kappa_2(A)$.

The loss of orthogonality ω of columns of $C = AV$ clearly depends linearly on $\kappa_2(A)$ as predicted by (17). Its upper bound given by term $2\kappa_2(A)\|\delta S\|_2$ is an overestimate as is usually the case, but the difference of approximately two orders of magnitude is acceptable.

Results of numerical experiments for the geometrically distributed SVs are depicted in Fig. 3 and Fig. 4 for $k = 1$ and $k = 6$, respectively.

Surprisingly, we can observe a substantial difference in the behavior of $\|\delta S\|_2$ as compared to the arithmetically distributed SVs. Regardless to k , the value of $\|\delta S\|_2$ depends on $\kappa_2(A)$ and increases with increasing $\kappa_2(A)$. This increase is substantial for ill-conditioned matrices with $\kappa_2(A) \in \{10^4, 10^6, 10^8\}$, i.e., for matrices with the GMI in interval $[201, 500]$. Moreover, for these ill-conditioned matrices one observes a large dispersion in the values of $\|\delta S\|_2$ as well as of ω in the case of using 1 HI (see Fig. 3), whereas those parameters are much more stabilized when using 6 HI (see Fig. 4).

Note that with an increasing $\kappa_2(A)$ one gets progressively tighter clusters of SVs of a matrix A toward the smallest SV $\sigma_n = \kappa_2^{-1}(A)$. Therefore it seems that the MATLAB function `eig()`, which implements the DCA for the EVD of symmetric matrices, does not deliver the eigenpairs of sufficient quality in the case of tightly clustered eigenvalues. Note, however, that the computed matrix of eigenvectors V is still numerically orthogonal to a very high level regardless to $\kappa_2(A)$, so it is possible to set $\|\delta V\|_2 \approx 0$ again. The loss of orthogonality of columns of $C = AV$ is still linearly proportional to $\kappa_2(A)$ in accordance with (17)

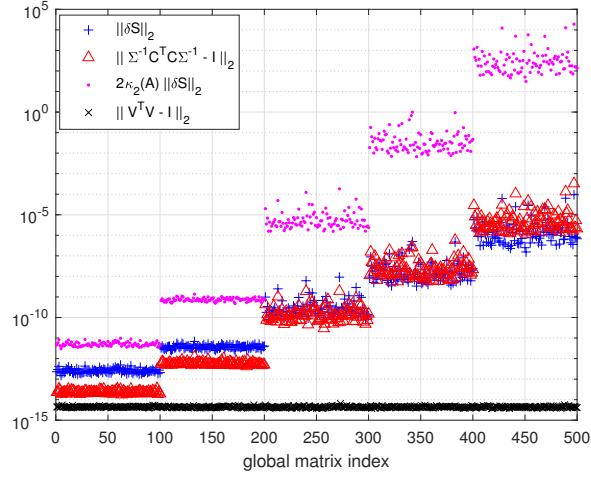


Fig. 3. Results using 1 Halley's iteration and a geometric sequence of SVs

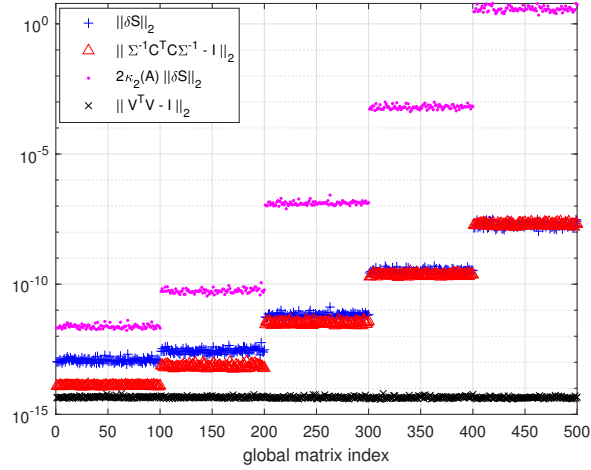


Fig. 4. Results using 6 Halley's iterations and a geometric sequence of SVs

and is comparable to that for the arithmetically distributed SVs (compare Fig. 4 with Fig. 2). Note that the values of $\|\delta S\|_2$ and ω often overlap—especially for ill-conditioned matrices with the GMI larger than 200. Moreover, for ill-conditioned matrices, the values of upper bound $2\kappa_2(A)\|\delta S\|_2$ give a huge overestimate of ω due to the relatively large values of $\|\delta S\|_2$ and are not realistic at all.

6 Conclusions

We have shown that, under reasonable assumptions, the computation $\hat{C} = \mathcal{F}(\hat{V}A)$ changes all singular triplets of a column-graded matrix A by only a small relative amount. It is easy to see that the same conclusion is valid also for the computation $\mathcal{F}(A\hat{V})$ with a row-graded matrix $A = DB$. Hence, our approach of preconditioning the one-sided block Jacobi algorithm, which was described in [1], is numerically justified in the sense, that the Jacobi algorithm applied to the preconditioned matrix $\mathcal{F}(\hat{V}A)$ (or $\mathcal{F}(A\hat{V})$) computes with a high relative accuracy all singular triplets that differ relatively from the singular triplets of A only by a small amount.

Let us emphasize that in our application the numerically orthogonal matrix $\hat{V}$ is very special: the matrix product $\hat{C} = \mathcal{F}(\hat{V}A)$ (or $\hat{C} = \mathcal{F}(A\hat{V})$) should be ‘close’ to the matrix of scaled right (or left) singular vectors of A , so that $\hat{C}$ should have nearly orthogonal columns. Numerical experiments in MATLAB have shown, that the loss of orthogonality in the columns of $\hat{C}$ is proportional to $\kappa_2(A)$, which is in accordance with the upper bound in (17). However, for ill-conditioned matrices with $\kappa_2(A) \geq 10^4$ and geometrically distributed SVs in the interval $[\kappa_2^{-1}(A), 1]$, the computed eigenvalues and eigenvectors of the polar Hermitian factor using the MATLAB function `eig()` (which is based on the DCA) are of insufficient quality—presumably due to a tight clustering of SVs toward $\sigma_n = \kappa_2^{-1}(A)$. Such a degradation was not observed in the case of arithmetically distributed SVs with a constant gap between neighboring SVs. This topic deserves further research.

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