On convergence to singular triplets in the two-sided block-Jacobi SVD algorithm with dynamic ordering: Part I

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On convergence to singular triplets in the two-sided block-Jacobi SVD algorithm with dynamic ordering: Part I

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Abstract. *We study the convergence towards singular triplets in the serial two-sided block-Jacobi SVD algorithm with dynamic ordering. This Part I contains the proof of convergence of diagonal elements of the iterated matrix towards singular values. Furthemore, we provide the proof of convergence of two computed vector sequences towards the left and right singular vector that correspond to a simple singular value. An interesting by-product is the generalization of the real* $\sin\Theta$ *theorem in [12, Theorem 11.7.1] to the complex SVD case.*

1 Introduction

In the analysis of convergence of the two-sided scalar or block-Jacobi algorithm for the computation of the singular value decomposition (SVD) of a general matrix, most papers deal with the convergence of the off-diagonal Frobenius norm of an iterated matrix to zero.

Here we consider the block version of the classical SVD Jacobi method, in which two off-diagonal blocks with the largest sum of the squares of their Frobenius norms are zeroed in each serial iteration step. The asymptotic quadratic convergence of the off-diagonal Frobenius norm to zero has been proven in [11] for the serial and parallel algorithm. In this paper, we study the convergence towards singular triplets of a given general matrix A.

We start with some preliminaries in subsection 2.1 that are needed for the theory developed subsequently. Next we show that an iterated matrix $A^{(k)}$ indeed converges to a fixed diagonal matrix Σ and its diagonal elements are the singular values of an initial matrix A. This is proved

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in subsection 2.2 regardless of the multiplicity or presence of clusters of eigenvalues, if a block partition of A into a $w \times w$ block structure ensures that each multiple singular values or a cluster of singular values is confined to one diagonal block.

Regarding the notation, the identity matrix of order n is denoted by I_n and the $m \times n$ zero matrix by O_{mn}. For a square matrix A, $\mathrm{off}(A)$ denotes a matrix consisting of its off-diagonal elements, A^{H} its Hermitian conjugate, $\|A\|_{\mathsf{F}}$ its Frobenius norm and $\|A\|_2$ its 2-norm. For a matrix A, we denote its smallest and largest real singular value by $\sigma_{\min}(A)$ and $\sigma_{\max}(A)$, respectively. The bold font is used for vectors (e.g., $\mathbf{u}$), whereas projectors and index sets are denoted by calligraphic symbols (e.g., $\mathcal{P}$, $\mathcal{I}$). Finally, for two integers i and j, $i \leq j$, the symbol $i : j$ denotes the set of all integers $i, i+1, \ldots, j$.

2 Convergence analysis

2.1 Preliminaries

The SVD of a general matrix $A = A^{(0)} \in \mathbb{C}^{m \times n}$, $m \geq n$, is defined as the decomposition $A = U(\Sigma, 0^T)^T V^{\mathsf{H}}$, where U (of size $m \times m$) and V (of size $n \times n$) is the unitary matrix of left and right singular vectors, respectively, and Σ is the $n \times n$ diagonal matrix with real non-negative diagonal elements $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_n \geq 0$.

In the convergence analysis of any SVD algorithm, it is sufficient to consider only square matrices of full rank. If an original matrix is rectangular (e.g., with $m > n$) with $\mathrm{rank}(A) = r \leq n$, one can initially compute its QR decomposition with column pivoting (c.f. [4, 5, 6, 7]), which reveals the rank defficiency of A by moving $n - r$ zero elements on the main diagonal of the factor R of size n down to its lower right corner. The subsequent LQ factorization of R results in the lower triangular matrix L with full rank r placed in the upper left corner and bordered by zero rows and columns up to the size n. Hence, the singular triplets for zero singular values can be obtained after application of two finite decompositions, and the iterative SVD algorithm is applied only to L of size r. The SVD of A is then reconstructed in an obvious way. Consequently, we assume in the following that a matrix A is square of size n and of full rank, i.e., $\sigma_n > 0$.

Firstly, we recall several theorems and lemmas to be used in the following subsections. In the following, we consider applying the two-sided block-Jacobi SVD algorithm to a matrix $A = A^{(0)} \in \mathbb{C}^{n \times n}$ partitioned into a $w \times w$ block structure ($w > 2$). To keep the notation simple, we assume that n is divisible by w and consider only equally sized blocks of size $\ell \times \ell$, where $\ell = n/w$. When n is not divisible by w, one can border the matrix with zero rows and columns up to the nearest multiple of w and add ones on the prolonged part of main diagonal. Then the SVD of an original matrix can be recovered from that of the bordered one easily. It should also be stressed that all subsequent theorems and lemmas can be proved for any general matrix partition $\{n_i\}_{i=1}^{w}$ such that $\sum_{i=1}^{w} n_i = n$ and the jth diagonal block is square of order $n_j \times n_j$.

The iterated matrix obtained after the kth step is denoted by $A^{(k)}$. We also assume that the diagonal blocks of A are diagonalized before the first step and the diagonal elements in each diagonal block are ordered non-increasingly. Hence, the diagonal blocks of $A^{(k)}$ remain diagonal throughout the whole computation.

At iteration step k the two-sided block-Jacobi SVD algorithm proceeds as follows. We choose two off-diagonal blocks of $A^{(k)}$, say, $A^{(k)}_{X_kY_k}$ and $A^{(k)}_{Y_kX_k}$ (X_k, Y_k integers, $X_k < Y_k$), with the largest sum of the squares of their Frobenius norms. This choice is called the *dynamic ordering* in [11]. These two off-diagonal blocks are zeroed by a two-sided unitary transformation

$$(\hat{U}^{(k)})^{\mathsf{H}} A^{(k)} \hat{V}^{(k)} = A^{(k+1)},$$

where the $n \times n$ unitary matrices $\hat{U}^{(k)}$ and $\hat{V}^{(k)}$ are the matrices of local left and right singular vectors from a 2×2 block subproblem, respectively, embedded into the identity matrix I_n of order n. Four blocks of $\hat{U}^{(k)}$ and $\hat{V}^{(k)}$, each of order ℓ, that are different from blocks of I_n can be chosen so that

$$\begin{pmatrix} \tilde{U}^{(k)}_{X_kX_k} & \tilde{U}^{(k)}_{X_kY_k} \\ \tilde{U}^{(k)}_{Y_kX_k} & \tilde{U}^{(k)}_{Y_kY_k} \end{pmatrix}^{\mathsf{H}} \begin{pmatrix} A^{(k)}_{X_kX_k} & A^{(k)}_{X_kY_k} \\ A^{(k)}_{Y_kX_k} & A^{(k)}_{Y_kY_k} \end{pmatrix} \begin{pmatrix} \tilde{V}^{(k)}_{X_kX_k} & \tilde{V}^{(k)}_{X_kY_k} \\ \tilde{V}^{(k)}_{Y_kX_k} & \tilde{V}^{(k)}_{Y_kY_k} \end{pmatrix} = \begin{pmatrix} A^{(k+1)}_{X_kX_k} & 0 \\ 0 & A^{(k+1)}_{Y_kY_k} \end{pmatrix}, \tag{1}$$

where the diagonal blocks $A^{(k+1)}_{X_kX_k}$ and $A^{(k+1)}_{Y_kY_k}$ are square, diagonal matrices of order ℓ with real nonnegative diagonal elements (local singular values).

Let us define

$$\tilde{U}^{(k)} \equiv \begin{pmatrix} \tilde{U}^{(k)}_{X_kX_k} & \tilde{U}^{(k)}_{X_kY_k} \\ \tilde{U}^{(k)}_{Y_kX_k} & \tilde{U}^{(k)}_{Y_kY_k} \end{pmatrix}, \quad \tilde{V}^{(k)} \equiv \begin{pmatrix} \tilde{V}^{(k)}_{X_kX_k} & \tilde{V}^{(k)}_{X_kY_k} \\ \tilde{V}^{(k)}_{Y_kX_k} & \tilde{V}^{(k)}_{Y_kY_k} \end{pmatrix}, \tag{2}$$

and

$$\tilde{A}^{(k)} \equiv \begin{pmatrix} A^{(k)}_{X_kX_k} & A^{(k)}_{X_kY_k} \\ A^{(k)}_{Y_kX_k} & A^{(k)}_{Y_kY_k} \end{pmatrix}, \quad \tilde{\Sigma}^{(k+1)} \equiv \begin{pmatrix} A^{(k+1)}_{X_kX_k} & 0 \\ 0 & A^{(k+1)}_{Y_kY_k} \end{pmatrix}. \tag{3}$$

Because Eq. (1) is the SVD of the matrix $\tilde{A}^{(k)}$, the matrix $\tilde{U}^{(k)}$ and $\tilde{V}^{(k)}$ is the unitary matrix of left and right singular vectors of $\tilde{A}^{(k)}$, respectively.

Next, we *scale* the matrix $\tilde{V}^{(k)}$ of local right singular vectors as follows. Write the ith diagonal element of $\tilde{V}^{(k)}$ in polar coordinates as $\tilde{v}^{(k)}_{ii} = |\tilde{v}^{(k)}_{ii}| \exp(\iota\theta^{(k)}_i)$. Construct the diagonal matrix

$$D^{(k)}_V = \operatorname{diag}[\exp(-\iota\theta^{(k)}_1), \exp(-\iota\theta^{(k)}_2), \ldots, \exp(-\iota\theta^{(k)}_{2\ell})],$$

and compute the updates:

$$\tilde{U}^{(k)} \leftarrow \tilde{U}^{(k)} D^{(k)}_V, \quad \tilde{V}^{(k)} \leftarrow \tilde{V}^{(k)} D^{(k)}_V. \tag{4}$$

After the updates, the matrix $\tilde{V}^{(k)}$ has *real, nonnegative elements on its diagonal*, while those of $\tilde{U}^{(k)}$ remain complex. Note that the *same* diagonal matrix $D^{(k)}_V$ has to be used in Eq. (4). Otherwise, the local SVD, $\tilde{A}^{(k)}\tilde{V}^{(k)} = \tilde{U}^{(k)}\tilde{\Sigma}^{(k+1)}$, would not be preserved. In other words, it is not possible to scale *both* matrices $\tilde{V}^{(k)}$ and $\tilde{U}^{(k)}$ for getting real nonnegative elements on their main diagonals *simultaneously* without violating their mutual relation in the local SVD of $\tilde{A}^{(k)}$.

This scaling of local right singular vectors will be important in the proof of Theorem 4 in subsection 2.3.

At the same time, the matrices $\hat{U}^{(k)}$ and $\hat{V}^{(k)}$, i.e., the embeddings of $\tilde{U}^{(k)}$ and $\tilde{V}^{(k)}$, respectively, are accumulated as

$$U^{(k+1)} = U^{(k)}\hat{U}^{(k)}, \quad V^{(k+1)} = V^{(k)}\hat{V}^{(k)}, \tag{5}$$

with $U^{(0)} = V^{(0)} = I_n$. Hence, at the beginning of iteration step $k+1$, the two-sided unitary transformation of the original matrix A is of the form

$$(U^{(k+1)})^{\mathsf{H}} A V^{(k+1)} = A^{(k+1)}, \quad \text{or} \quad AV^{(k+1)} = U^{(k+1)}A^{(k+1)}. \tag{6}$$

As shown in [11, Eq.(5)], the off-diagonal Frobenius norm of $A^{(k+1)}$ converges to zero, i.e.,

$$\|\mathrm{off}(A^{(k+1)})\|_{\mathsf{F}}^2 \leq \alpha \|\mathrm{off}(A^{(k)})\|_{\mathsf{F}}^2, \quad \text{where} \quad \alpha \equiv 1 - \frac{2}{w(w-1)} < 1. \tag{7}$$

Specifically, defining $S(A) \equiv \|\mathrm{off}(A)\|_{\mathsf{F}}^2$, we have

$$\|\mathrm{off}(A^{(k)})\|_{\mathsf{F}}^2 \leq S(A)\,\alpha^k, \tag{8}$$

i.e., the square of the off-diagonal Frobenius norm decreases at least as fast as the geometric sequence with the quotient α. The next theorem and its corollary will be used to prove the convergence of diagonal elements of $A^{(k)}$.

Theorem 1 (Hoffman-Wielandt theorem [9]) *Let $B,\ C \in \mathbb{C}^{n\times n}$ with their respective singular values $\{\sigma_i(B)\}_{i=1}^n$ and $\{\sigma_i(C)\}_{i=1}^n$. Also, let $\mathcal{S}_n$ denote the permutation group of $\{1, 2, \ldots, n\}$. Then,*

$$\min_{\tau\in\mathcal{S}_n} \sum_{i=1}^{n} |\sigma_i(B) - \sigma_{\tau(i)}(C)|^2 \leq \|B - C\|_{\mathsf{F}}^2.$$

Corollary 1 *Let $\{\sigma_i(B)\}_{i=1}^n$ and $\{\sigma_i(C)\}_{i=1}^n$ be ordered non-increasingly (or non-decreasingly). Then,*

$$\sum_{i=1}^{n} |\sigma_i(B) - \sigma_i(C)|^2 \leq \|B - C\|_{\mathsf{F}}^2.$$

The next theorem is a generalization of the real $\sin\Theta$ theorem in [12, Theorem 11.7.1] to the complex SVD case. Here, for two vectors $\mathbf{0} \neq \mathbf{x}, \mathbf{y} \in \mathbb{C}^m$ for which the inner product $\mathbf{x}^{\mathsf{H}}\mathbf{y}$ is real, the angle $\angle(\mathbf{y}, \mathbf{x})$ between them is defined as a real number θ, $0 \leq \theta \leq \pi$, such that $\cos\theta = \mathbf{x}^{\mathsf{H}}\mathbf{y}/(\|\mathbf{x}\|\,\|\mathbf{y}\|) \in \mathbb{R}$, $-1 \leq \cos\theta \leq 1$.

Theorem 2 *Let $B \in \mathbb{C}^{m\times m}$, and let $\mathbf{x}, \mathbf{y} \in \mathbb{C}^m$ be two vectors with $\|\mathbf{x}\| = \|\mathbf{y}\| = 1$. Define the Rayleigh quotient for the SVD as $\varrho \equiv \mathbf{x}^{\mathsf{H}}B\mathbf{y} \in \mathbb{C}$, and two residuals: $\mathbf{r}(\mathbf{x}, \mathbf{y}) \equiv B\mathbf{y} - |\varrho|\mathbf{x}$, $\mathbf{s}(\mathbf{x}, \mathbf{y}) \equiv B^{\mathsf{H}}\mathbf{x} - |\varrho|\mathbf{y}$. Let σ_i be the singular value of B that is closest to $|\varrho|$ with $\mathbf{u}_i$ and $\mathbf{v}_i$ being the corresponding left and right singular vector, respectively. Additionally, let $\mathbf{u}_i^{\mathsf{H}}\mathbf{x} \in \mathbb{R}$ and $\mathbf{v}_i^{\mathsf{H}}\mathbf{y} \in \mathbb{R}$. Let $\varphi \equiv \angle(\mathbf{x}, \mathbf{u}_i)$, $\theta \equiv \angle(\mathbf{y}, \mathbf{v}_i)$ and $\mathrm{gap}(\varrho) \equiv \min_{\sigma_j\neq\sigma_i} |\sigma_j - |\varrho||$. Then the following inequality holds:*

$$\sqrt{\sin^2\varphi + \sin^2\theta} \leq \frac{\sqrt{\|\mathbf{r}(\mathbf{x}, \mathbf{y})\|^2 + \|\mathbf{s}(\mathbf{x}, \mathbf{y})\|^2}}{\mathrm{gap}(\varrho)}. \tag{9}$$

Proof: If $\mathbf{x} = \pm\mathbf{u}_i$ and $\mathbf{y} = \pm\mathbf{v}_i$, there is nothing to prove, because $\mathbf{r}(\mathbf{x},\mathbf{y}) = \mathbf{s}(\mathbf{x},\mathbf{y}) = \mathbf{0}$ and $\varphi = \theta = 0$. Next, three cases will be analyzed.

a) Case $\mathbf{x} \neq \pm\mathbf{u}_i$ *and* $\mathbf{v} \neq \pm\mathbf{v}_i$: The linear subspaces $\text{span}(\mathbf{u}_i, \mathbf{x})$ and $\text{span}(\mathbf{v}_i, \mathbf{y})$ are 2-dimensional, and using the approach in [17, Thm.3] the vectors $\mathbf{x}$ and $\mathbf{y}$ can be decomposed as follows:

$$\mathbf{x} = \cos\varphi\, \mathbf{u}_i + \sin\varphi\, \mathbf{z}, \quad \mathbf{y} = \cos\theta\, \mathbf{v}_i + \sin\theta\, \mathbf{w},$$

where $\mathbf{z}^{\mathsf{H}}\mathbf{u}_i = 0$, $\|\mathbf{z}\| = 1$ and $\mathbf{w}^{\mathsf{H}}\mathbf{v}_i = 0$, $\|\mathbf{w}\| = 1$. Since $B\mathbf{v}_i = \sigma_i\mathbf{u}_i$ and $B^{\mathsf{H}}\mathbf{u}_i = \sigma_i\mathbf{v}_i$, one has:

$$\begin{aligned} \mathbf{r}(\mathbf{x},\mathbf{y}) &= \sigma_i \cos\theta\, \mathbf{u}_i + \sin\theta\, B\mathbf{w} - |\varrho|\cos\varphi\, \mathbf{u}_i - |\varrho|\sin\varphi\, \mathbf{z}, \\ \mathbf{s}(\mathbf{x},\mathbf{y}) &= \sigma_i \cos\varphi\, \mathbf{v}_i + \sin\varphi\, B^{\mathsf{H}}\mathbf{z} - |\varrho|\cos\theta\, \mathbf{v}_i - |\varrho|\sin\theta\, \mathbf{w}. \end{aligned} \tag{10}$$

The sets of left and right singular vectors of B create two orthonormal bases in $\mathbb{C}^m$. Recall that $\mathbf{z}$ is orthogonal to $\mathbf{u}_i$, and $\mathbf{w}$ is orthogonal to $\mathbf{v}_i$. Hence, there exist coefficients α_j, $\beta_j \in \mathbb{C}$, $1 \le j \le m$, $j \neq i$, such that $\mathbf{w} = \sum_{j=1,j\neq i}^{m} \alpha_j \mathbf{v}_j$ with $\sum_{j=1,j\neq i}^{m} |\alpha_j|^2 = 1$, and $\mathbf{z} = \sum_{j=1,j\neq i}^{m} \beta_j \mathbf{u}_j$ with $\sum_{j=1,j\neq i}^{m} |\beta_j|^2 = 1$. Moreover, $B\mathbf{w} = \sum_{j=1,j\neq i}^{m} \alpha_j\sigma_j\mathbf{u}_j$ and $B^{\mathsf{H}}\mathbf{z} = \sum_{j=1,j\neq i}^{m} \beta_j\sigma_j\mathbf{v}_j$. Consequently, Eq. (10) can be written as

$$\begin{aligned} \mathbf{r}(\mathbf{x},\mathbf{y}) &= (\sigma_i\cos\theta - |\varrho|\cos\varphi)\mathbf{u}_i + \sum_{j=1,j\neq i}^{m} (\alpha_j\sigma_j\sin\theta - |\varrho|\beta_j\sin\varphi)\mathbf{u}_j, \\ \mathbf{s}(\mathbf{x},\mathbf{y}) &= (\sigma_i\cos\varphi - |\varrho|\cos\theta)\mathbf{v}_i + \sum_{j=1,j\neq i}^{m} (\beta_j\sigma_j\sin\varphi - |\varrho|\alpha_j\sin\theta)\mathbf{v}_j, \end{aligned}$$

and, using the theorem of Pythagoras, the squares of residual norms are of the form

$$\begin{aligned} \|\mathbf{r}(\mathbf{x},\mathbf{y})\|^2 &= (\sigma_i\cos\theta - |\varrho|\cos\varphi)^2 + \sum_{j=1,j\neq i}^{m} |\alpha_j\sigma_j\sin\theta - |\varrho|\beta_j\sin\varphi|^2, \\ \|\mathbf{s}(\mathbf{x},\mathbf{y})\|^2 &= (\sigma_i\cos\varphi - |\varrho|\cos\theta)^2 + \sum_{j=1,j\neq i}^{m} |\beta_j\sigma_j\sin\varphi - |\varrho|\alpha_j\sin\theta|^2. \end{aligned} \tag{11}$$

After omitting the first terms on the right-hand side of Eq. (11), which are real and nonnegative, one gets the first lower bound for each residual:

$$\begin{aligned} \|\mathbf{r}(\mathbf{x},\mathbf{y})\|^2 &\ge \sum_{j=1,j\neq i}^{m} |\alpha_j\sigma_j\sin\theta - |\varrho|\beta_j\sin\varphi|^2, \\ \|\mathbf{s}(\mathbf{x},\mathbf{y})\|^2 &\ge \sum_{j=1,j\neq i}^{m} |\beta_j\sigma_j\sin\varphi - |\varrho|\alpha_j\sin\theta|^2. \end{aligned} \tag{12}$$

Each term in each sum of Eq. (12) contains complex numbers α_j and β_j, which are combined with real constants. Noting that for any complex number γ, $|\gamma|^2 = \gamma\bar{\gamma}$, where $\bar{\gamma}$ is the complex conjugate number to γ, one has:

$$\begin{aligned} |\alpha_j\sigma_j\sin\theta - |\varrho|\beta_j\sin\varphi|^2 &= (\alpha_j\sigma_j\sin\theta - |\varrho|\beta_j\sin\varphi)\,(\bar{\alpha}_j\sigma_j\sin\theta - |\varrho|\bar{\beta}_j\sin\varphi) \\ &= |\alpha_j|^2\sigma_j^2\sin^2\theta + |\beta_j|^2|\varrho|^2\sin^2\varphi - (\bar{\alpha}_j\beta_j + \alpha_j\bar{\beta}_j)|\varrho|\,\sigma_j\sin\theta\,\sin\varphi \\ &= |\alpha_j|^2\sigma_j^2\sin^2\theta + |\beta_j|^2|\varrho|^2\sin^2\varphi - 2\,\text{Re}(\alpha_j\bar{\beta}_j)\,|\varrho|\,\sigma_j\sin\theta\,\sin\varphi, \end{aligned}$$

where $\mathrm{Re}(\gamma)$ is the real part of a complex number γ.

Similarly,

$$|\beta_j\sigma_j \sin\varphi - |\varrho|\alpha_j \sin\theta|^2 = (\beta_j\sigma_j \sin\varphi - |\varrho|\alpha_j \sin\theta)\,(\bar{\beta}_j\sigma_j \sin\varphi - |\varrho|\bar{\alpha}_j \sin\theta)$$
$$= |\alpha_j|^2|\varrho|^2 \sin^2\theta + |\beta_j|^2\sigma_j^2 \sin^2\varphi - 2\,\mathrm{Re}(\alpha_j\bar{\beta}_j)\,|\varrho|\,\sigma_j \sin\theta\,\sin\varphi.$$

Hence, the sum of both inequalities in Eq. (12) gives:

$$\begin{aligned}
\|\mathbf{r}(\mathbf{x},\mathbf{y})\|^2 + \|\mathbf{s}(\mathbf{x},\mathbf{y})\|^2 \geq& \sum_{j=1,j\neq i}^{m} (|\alpha_j|^2\sigma_j^2 \sin^2\theta + |\alpha_j|^2|\varrho|^2 \sin^2\theta) \\
&+ \sum_{j=1,j\neq i}^{m} (|\beta_j|^2\sigma_j^2 \sin^2\varphi + |\beta_j|^2|\varrho|^2 \sin^2\varphi) \\
&-4 \sum_{j=1,j\neq i}^{m} \mathrm{Re}(\alpha_j\bar{\beta}_j)\,|\varrho|\,\sigma_j \sin\theta\,\sin\varphi \\
=& \sum_{j=1,j\neq i}^{m} |\alpha_j|^2(\sigma_j - |\varrho|)^2 \sin^2\theta + 2\sum_{j=1,j\neq i}^{m} |\alpha_j|^2\sigma_j|\varrho| \sin^2\theta \\
&+ \sum_{j=1,j\neq i}^{m} |\beta_j|^2(\sigma_j - |\varrho|)^2 \sin^2\varphi + 2\sum_{j=1,j\neq i}^{m} |\beta_j|^2\sigma_j|\varrho| \sin^2\varphi \\
&-4 \sum_{j=1,j\neq i}^{m} \mathrm{Re}(\alpha_j\bar{\beta}_j)\,|\varrho|\,\sigma_j \sin\theta\,\sin\varphi.
\end{aligned}$$

But

$$\begin{aligned}
\mathrm{Re}(\alpha_j\bar{\beta}_j)\,\sin\theta\,\sin\varphi &\leq |\mathrm{Re}(\alpha_j\bar{\beta}_j)|\,|\sin\theta|\,|\sin\varphi| \leq |\alpha_j\bar{\beta}_j|\,|\sin\theta|\,|\sin\varphi| \\
&= |\alpha_j||\beta_j|\,|\sin\theta|\,|\sin\varphi|,
\end{aligned}$$

so that

$$\begin{aligned}
\|\mathbf{r}(\mathbf{x},\mathbf{y})\|^2 + \|\mathbf{s}(\mathbf{x},\mathbf{y})\|^2 \geq& \sum_{j=1,j\neq i}^{m} |\alpha_j|^2(\sigma_j - |\varrho|)^2 \sin^2\theta \\
&+ \sum_{j=1,j\neq i}^{m} |\beta_j|^2(\sigma_j - |\varrho|)^2 \sin^2\varphi \\
&+2 \sum_{j=1,j\neq i}^{m} |\varrho|\,\sigma_j\,\big(|\alpha_j|^2 \sin^2\theta - 2|\alpha_j||\beta_j||\sin\theta||\sin\varphi| + |\beta_j|^2 \sin^2\varphi\big) \\
\geq& \min_{\sigma_j\neq\sigma_i} (\sigma_j - |\varrho|)^2(\sin^2\theta + \sin^2\varphi) + 2|\varrho| \sum_{j=1,j\neq i}^{m} \sigma_j\,(|\alpha_j||\sin\theta| - |\beta_j||\sin\varphi|)^2 \\
\geq& [\mathrm{gap}(\varrho)]^2\,(\sin^2\theta + \sin^2\varphi),
\end{aligned}$$

where, in the first inequality, we have used $\sum_{j=1,j\neq i}^{m} |\alpha_j|^2 = \sum_{j=1,j\neq i}^{m} |\beta_j|^2 = 1$. Hence, the bound in Eq. (9) is proved.

b) Case $\mathbf{x} = \pm\mathbf{u}_i$ *and* $\mathbf{v} \neq \pm\mathbf{v}_i$: Here $\sin\varphi = 0$, and $\varphi = 0$ for $\mathbf{x} = +\mathbf{u}_i$ or $\varphi = \pi$ for $\mathbf{x} = -\mathbf{u}_i$. In either case, the vector $\mathbf{z}$ can be chosen as $\mathbf{u}_k$ for arbitrary $k \neq i$. Then the lower bound for $\|\mathbf{r}(\mathbf{x},\mathbf{y})\|^2 + \|\mathbf{s}(\mathbf{x},\mathbf{y})\|^2$ reduces to $[\mathrm{gap}(\varrho)]^2 \sin^2\theta$, which is exactly Eq. (9) with $\sin\varphi = 0$.

c) Case $\mathbf{x} \neq \pm\mathbf{u}_i$ *and* $\mathbf{v} = \pm\mathbf{v}_i$: Consequently, $\sin\theta = 0$ and $\theta = 0$ for $\mathbf{y} = +\mathbf{v}_i$ or $\theta = \pi$ for $\mathbf{y} = -\mathbf{v}_i$. In analogy to the case *b)*, the vector $\mathbf{w}$ can be chosen as $\mathbf{v}_k$ for arbitrary $k \neq i$. Then the lower bound for $\|\mathbf{r}(\mathbf{x},\mathbf{y})\|^2 + \|\mathbf{s}(\mathbf{x},\mathbf{y})\|^2$ reduces to $[\mathrm{gap}(\varrho)]^2 \sin^2\varphi$, which is exactly Eq. (9) with $\sin\theta = 0$. □

The assumption about two real scalar products in Theorem 2 is very special. In next two corollaries, these assumptions will be replaced by one or two complex scalar products. In the next corollary, the first "mixed" case is analyzed with one real and one complex scalar product.

Corollary 2 *Using the notation of Theorem 2 (including its proof), let* $\mathbf{u}_i^{\mathsf{H}}\mathbf{x} \in \mathbb{C}$ *and* $\mathbf{v}_i^{\mathsf{H}}\mathbf{y} \in \mathbb{R}$, *so that only the angle* θ *is well defined. Then*

$$\sqrt{|\mathbf{z}^{\mathsf{H}}\mathbf{x}|^2 + \sin^2\theta} \leq \frac{\sqrt{\|\mathbf{r}(\mathbf{x},\mathbf{y})\|^2 + \|\mathbf{s}(\mathbf{x},\mathbf{y})\|^2}}{\mathrm{gap}(\varrho)}, \tag{13}$$

where $\mathbf{x} \in \mathrm{span}(\mathbf{u}_i, \mathbf{z})$, $\mathbf{z}^{\mathsf{H}}\mathbf{u}_i = 0$ *and* $\|\mathbf{z}\| = 1$.

Proof: In this case, the decomposition of two approximating vectors $\mathbf{x}$ and $\mathbf{y}$ is given by

$$\begin{aligned} \mathbf{x} &= (\mathbf{u}_i^{\mathsf{H}}\mathbf{x})\mathbf{u}_i + (\mathbf{z}^{\mathsf{H}}\mathbf{x})\mathbf{z} = \mu\mathbf{u}_i + \nu\mathbf{z}, \\ \mathbf{y} &= \cos\theta\,\mathbf{v}_i + \sin\theta\,\mathbf{w}, \end{aligned}$$

where μ, $\nu \in \mathbb{C}$ and $|\mu|^2 + |\nu|^2 = 1$. Now, all derivations in the proof of Theorem 2 remain valid with $\cos\varphi$ replaced by μ and $\sin\varphi$ replaced by ν. Hence,

$$\|\mathbf{r}(\mathbf{x},\mathbf{y})\|^2 = |\sigma_i\cos\theta - |\varrho|\mu|^2 + \sum_{j=1, j\neq i}^{m} |\alpha_j\sigma_j\sin\theta - |\varrho|\beta_j\nu|^2,$$

$$\|\mathbf{s}(\mathbf{x},\mathbf{y})\|^2 = |\sigma_i\mu - |\varrho|\cos\theta|^2 + \sum_{j=1, j\neq i}^{m} |\sigma_j\beta_j\nu - |\varrho|\alpha_j\sin\theta|^2,$$

so that

$$\begin{aligned} \|\mathbf{r}(\mathbf{x},\mathbf{y})\|^2 &\geq \sum_{j=1, j\neq i}^{m} |\alpha_j\sigma_j\sin\theta - |\varrho|\beta_j\nu|^2, \\ \|\mathbf{s}(\mathbf{x},\mathbf{y})\|^2 &\geq \sum_{j=1, j\neq i}^{m} |\sigma_j\beta_j\nu - |\varrho|\alpha_j\sin\theta|^2. \end{aligned}$$

Using the substitution $\gamma_j = \beta_j\nu \in \mathbb{C}$,

$$\begin{aligned} |\alpha_j\sigma_j\sin\theta - |\varrho|\gamma_j|^2 &= (\alpha_j\sigma_j\sin\theta - |\varrho|\gamma_j)\,(\bar{\alpha}_j\sigma_j\sin\theta - |\varrho|\bar{\gamma}_j) \\ &= |\alpha_j|^2\sigma_j^2\sin^2\theta + |\gamma_j|^2|\varrho|^2 - (\bar{\alpha}_j\gamma_j + \alpha_j\bar{\gamma}_j)|\varrho|\,\sigma_j\sin\theta \\ &= |\alpha_j|^2\sigma_j^2\sin^2\theta + |\gamma_j|^2|\varrho|^2 - 2\,\mathrm{Re}(\alpha_j\bar{\gamma}_j)\,|\varrho|\,\sigma_j\sin\theta. \end{aligned}$$

Similarly,

$$\begin{aligned}|\sigma_j\gamma_j - |\varrho|\alpha_j\sin\theta|^2 &= (\sigma_j\gamma_j - |\varrho|\alpha_j\sin\theta)\,(\sigma_j\bar{\gamma}_j - |\varrho|\bar{\alpha}_j\sin\theta)\\ &= |\alpha_j|^2|\varrho|^2\sin^2\theta + \sigma_j^2|\gamma_j|^2 - 2\,\mathrm{Re}(\alpha_j\bar{\gamma}_j)\,|\varrho|\,\sigma_j\sin\theta.\end{aligned}$$

Hence,

$$\begin{aligned}\|\mathbf{r}(\mathbf{x},\mathbf{y})\|^2 + \|\mathbf{s}(\mathbf{x},\mathbf{y})\|^2 \geq \sum_{j=1,j\neq i}^{m} (|\alpha_j|^2\sigma_j^2\sin^2\theta + |\alpha_j|^2|\varrho|^2\sin^2\theta)\\ + \sum_{j=1,j\neq i}^{m} (|\gamma_j|^2\sigma_j^2 + |\gamma_j|^2|\varrho|^2)\\ -4\sum_{j=1,j\neq i}^{m} \mathrm{Re}(\alpha_j\bar{\gamma}_j)\,|\varrho|\,\sigma_j\sin\theta\\ = \sum_{j=1,j\neq i}^{m} |\alpha_j|^2(\sigma_j - |\varrho|)^2\sin^2\theta + 2\sum_{j=1,j\neq i}^{m} |\alpha_j|^2\sigma_j|\varrho|\sin^2\theta\\ + \sum_{j=1,j\neq i}^{m} |\gamma_j|^2(\sigma_j - |\varrho|)^2 + 2\sum_{j=1,j\neq i}^{m} |\gamma_j|^2\sigma_j|\varrho|\\ -4\sum_{j=1,j\neq i}^{m} \mathrm{Re}(\alpha_j\bar{\gamma}_j)\,|\varrho|\,\sigma_j\sin\theta.\end{aligned}$$

But

$$\begin{aligned}\mathrm{Re}(\alpha_j\bar{\gamma}_j)\,\sin\theta &\leq |\mathrm{Re}(\alpha_j\bar{\gamma}_j)|\,|\sin\theta| \leq |\alpha_j\bar{\gamma}_j|\,|\sin\theta|\\ &= |\alpha_j||\gamma_j|\,|\sin\theta|,\end{aligned}$$

so that

$$\begin{aligned}\|\mathbf{r}(\mathbf{x},\mathbf{y})\|^2 + \|\mathbf{s}(\mathbf{x},\mathbf{y})\|^2 \geq \sum_{j=1,j\neq i}^{m} |\alpha_j|^2(\sigma_j - |\varrho|)^2\sin^2\theta\\ + \sum_{j=1,j\neq i}^{m} |\gamma_j|^2(\sigma_j - |\varrho|)^2\\ +2\sum_{j=1,j\neq i}^{m} |\varrho|\,\sigma_j\,\left(|\alpha_j|^2\sin^2\theta - 2|\alpha_j||\gamma_j||\sin\theta| + |\gamma_j|^2\right)\\ \geq \min_{\sigma_j\neq\sigma_i}(\sigma_j - |\varrho|)^2(\sin^2\theta + |\nu|^2) + 2|\varrho|\sum_{j=1,j\neq i}^{m} \sigma_j\,(|\alpha_j||\sin\theta| - |\gamma_j|)^2\\ \geq [\mathrm{gap}(\varrho)]^2\,(\sin^2\theta + |\nu|^2),\end{aligned}$$

where, in the first inequality, we used the relation

$$\sum_{j=1,j\neq i}^{m} |\gamma_j|^2 = |\nu|^2\sum_{j=1,j\neq i}^{m} |\beta_j|^2 = |\nu|^2.$$

This proves the upper bound in Eq. (13). □

The second "mixed" case can be proved in the same way as Corollary 2. When $\mathbf{u}_i^{\mathsf{H}}\mathbf{x} \in \mathbb{R}$ and $\mathbf{v}_i^{\mathsf{H}}\mathbf{y} \in \mathbb{C}$, the approximating vectors have the decomposition

$$\begin{aligned} \mathbf{x} &= \cos\varphi\,\mathbf{u}_i + \sin\varphi\,\mathbf{z}, \\ \mathbf{y} &= (\mathbf{v}_i^{\mathsf{H}}\mathbf{y})\mathbf{v}_i + (\mathbf{w}^{\mathsf{H}}\mathbf{y})\mathbf{w}, \end{aligned}$$

and the bound in Eq. (13) changes to

$$\sqrt{\sin^2\varphi + |\mathbf{w}^{\mathsf{H}}\mathbf{y}|^2} \le \frac{\sqrt{\|\mathbf{r}(\mathbf{x},\mathbf{y})\|^2 + \|\mathbf{s}(\mathbf{x},\mathbf{y})\|^2}}{\operatorname{gap}(\varrho)}. \tag{14}$$

Finally, the next corollary provides the result for the most general case, i.e., when both scalar products are complex.

Corollary 3 *Using the notation of Theorem 2 (including its proof), let* $\mathbf{u}_i^{\mathsf{H}}\mathbf{x} \in \mathbb{C}$ *and* $\mathbf{v}_i^{\mathsf{H}}\mathbf{y} \in \mathbb{C}$. *Then*

$$\sqrt{|\mathbf{z}^{\mathsf{H}}\mathbf{x}|^2 + |\mathbf{w}^{\mathsf{H}}\mathbf{y}|^2} \le \frac{\sqrt{\|\mathbf{r}(\mathbf{x},\mathbf{y})\|^2 + \|\mathbf{s}(\mathbf{x},\mathbf{y})\|^2}}{\operatorname{gap}(\varrho)}, \tag{15}$$

where $\mathbf{x} \in \operatorname{span}(\mathbf{u}_i, \mathbf{z})$, $\mathbf{z}^{\mathsf{H}}\mathbf{u}_i = 0$, $\|\mathbf{z}\| = 1$, *and* $\mathbf{y} \in \operatorname{span}(\mathbf{v}_i, \mathbf{w})$, $\mathbf{w}^{\mathsf{H}}\mathbf{v}_i = 0$, $\|\mathbf{w}\| = 1$.

Proof: Write the decomposition of two approximating vectors $\mathbf{x}$ and $\mathbf{y}$ by

$$\begin{aligned} \mathbf{x} &= (\mathbf{u}_i^{\mathsf{H}}\mathbf{x})\mathbf{u}_i + (\mathbf{z}^{\mathsf{H}}\mathbf{x})\mathbf{z} = \mu\mathbf{u}_i + \nu\mathbf{z}, \\ \mathbf{y} &= (\mathbf{v}_i^{\mathsf{H}}\mathbf{y})\mathbf{v}_i + (\mathbf{w}^{\mathsf{H}}\mathbf{y})\mathbf{w} = \eta\mathbf{v}_i + \zeta\mathbf{w}, \end{aligned}$$

where $\mu, \nu, \eta, \zeta \in \mathbb{C}$, $|\mu|^2 + |\nu|^2 = 1$ and $|\eta|^2 + |\zeta|^2 = 1$. When compared with the proof of Corollary 2, it is easy to see that

$$\|\mathbf{r}(\mathbf{x},\mathbf{y})\|^2 = |\sigma_i\eta - |\varrho|\mu|^2 + \sum_{j=1,j\neq i}^{m} |\sigma_j\alpha_j\zeta - |\varrho|\beta_j\nu|^2,$$
$$\|\mathbf{s}(\mathbf{x},\mathbf{y})\|^2 = |\sigma_i\mu - |\varrho|\eta|^2 + \sum_{j=1,j\neq i}^{m} |\sigma_j\beta_j\nu - |\varrho|\alpha_j\zeta|^2.$$

Using the substitutions $\omega_j = \alpha_j\zeta$ and $\gamma_j = \beta_j\nu$, the first lower bounds for residuals can be written as

$$\begin{aligned} \|\mathbf{r}(\mathbf{x},\mathbf{y})\|^2 &\ge \sum_{j=1,j\neq i}^{m} |\sigma_j\omega_j - |\varrho|\gamma_j|^2, \\ \|\mathbf{s}(\mathbf{x},\mathbf{y})\|^2 &\ge \sum_{j=1,j\neq i}^{m} |\sigma_j\gamma_j - |\varrho|\omega_j|^2. \end{aligned}$$

Now, the proof continues exactly as that of Corollary 2 (however, without $\sin\theta$ and with ω_j instead of α_j), and its details are not repeated here. When finished, one gets the final lower bound:

$$
\begin{aligned}
\|\mathbf{r}(\mathbf{x},\mathbf{y})\|^2 + \|\mathbf{s}(\mathbf{x},\mathbf{y})\|^2 \geq \sum_{j=1, j\neq i}^{m} |\omega_j|^2(\sigma_j - |\varrho|)^2 \\
+ \sum_{j=1, j\neq i}^{m} |\gamma_j|^2(\sigma_j - |\varrho|)^2 \\
+2 \sum_{j=1, j\neq i}^{m} |\varrho|\, \sigma_j \, \left(|\omega_j|^2 - 2|\omega_j||\gamma_j| + |\gamma_j|^2\right) \\
\geq \min_{\sigma_j \neq \sigma_i} (\sigma_j - |\varrho|)^2 (|\nu|^2 + |\zeta|^2) + 2|\varrho| \sum_{j=1, j\neq i}^{m} \sigma_j \left(|\omega_j| - |\gamma_j|\right)^2 \\
\geq [\mathrm{gap}(\varrho)]^2 \left(|\nu|^2 + |\zeta|^2\right),
\end{aligned}
$$

where, in the first inequality, we used the relations

$$
\begin{aligned}
\sum_{j=1, j\neq i}^{m} |\omega_j|^2 = |\zeta|^2 \sum_{j=1, j\neq i}^{m} |\alpha_j|^2 = |\zeta|^2, \\
\sum_{j=1, j\neq i}^{m} |\gamma_j|^2 = |\nu|^2 \sum_{j=1, j\neq i}^{m} |\beta_j|^2 = |\nu|^2.
\end{aligned}
$$

This proves the assertion of the corollary. □

In summary, moving from Theorem 2 through Corollary 2 to Corollary 3, one can observe how the concept of "the angles between the approximating and approximated vectors" is replaced by the concept of "the components of approximating vectors that are orthogonal to the approximated vectors". The latter concept is certainly more general than the former one, because the angle between two vectors in $\mathbb{C}^m$ is not defined uniquely (except in the case of a real scalar product). In contrast, the orthogonality of two vectors can be defined in any vector space with some scalar product.

Note that the upper bound from Eq. (13) will be used in the proof of Theorem 4 in subsection 2.3.

Now we move to results that will be used in subsection 2.3. Let us consider a square 2×2 block matrix

$$
B = \begin{pmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{pmatrix},
$$

where square diagonal blocks may be of different sizes, and denote its SVD as

$$
\begin{pmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{pmatrix} \begin{pmatrix} V_{11} & V_{12} \\ V_{21} & V_{22} \end{pmatrix} = \begin{pmatrix} U_{11} & U_{12} \\ U_{21} & U_{22} \end{pmatrix} \begin{pmatrix} \Sigma_{11} & 0 \\ 0 & \Sigma_{22} \end{pmatrix}, \tag{16}
$$

where

$$
U = \begin{pmatrix} U_{11} & U_{12} \\ U_{21} & U_{22} \end{pmatrix} \quad \text{and} \quad V = \begin{pmatrix} V_{11} & V_{12} \\ V_{21} & V_{22} \end{pmatrix}
$$

are unitary and

$$\Sigma = \begin{pmatrix} \Sigma_{11} & 0 \\ 0 & \Sigma_{22} \end{pmatrix}$$

is diagonal with real nonnegative elements. Obviously, U and V can be chosen such that the diagonal elements of Σ are arranged in any particular order. The next lemma is used to bound the norm of the off-diagonal blocks of matrices of left and right singular vectors.

Lemma 1 *Assume that the diagonal elements of* Σ *are arranged in a non-increasing order. Further assume that* $\eta \equiv \sigma_{\min}(B_{11}) - \sigma_{\max}(B_{22}) > 0$ *and*

$$\sqrt{\|B_{12}\|_{\mathsf{F}}^2 + \|B_{21}\|_{\mathsf{F}}^2} < \eta.$$

Then

$$\left\| \begin{pmatrix} U_{21} \\ V_{21} \end{pmatrix} \right\|_{\mathsf{F}} \leq \frac{\sqrt{2}\sqrt{\|B_{12}\|_{\mathsf{F}}^2 + \|B_{21}\|_{\mathsf{F}}^2}}{\eta - \sqrt{\|B_{12}\|_{\mathsf{F}}^2 + \|B_{21}\|_{\mathsf{F}}^2}}. \tag{17}$$

Proof: In this proof we use the substitution $\omega \equiv \sqrt{\|B_{12}\|_{\mathsf{F}}^2 + \|B_{21}\|_{\mathsf{F}}^2}$. Let us write the complex conjugate of Eq. (16) as

$$\begin{pmatrix} B_{11}^{\mathsf{H}} & B_{21}^{\mathsf{H}} \\ B_{12}^{\mathsf{H}} & B_{22}^{\mathsf{H}} \end{pmatrix} \begin{pmatrix} U_{11} & U_{12} \\ U_{21} & U_{22} \end{pmatrix} = \begin{pmatrix} V_{11} & V_{12} \\ V_{21} & V_{22} \end{pmatrix} \begin{pmatrix} \Sigma_{11} & 0 \\ 0 & \Sigma_{22} \end{pmatrix}. \tag{18}$$

From Eqs. (16) and (18), let us extract two equations for the block $(2,1)$:

$$\begin{aligned} B_{22}V_{21} - U_{21}\Sigma_{11} &= -B_{21}V_{11} \\ B_{22}^{\mathsf{H}}U_{21} - V_{21}\Sigma_{11} &= -B_{12}^{\mathsf{H}}U_{11}, \end{aligned}$$

which can be written as the Sylvester equation for $(U_{21}^{\mathsf{T}}, V_{21}^{\mathsf{T}})^{\mathsf{T}}$:

$$-\begin{pmatrix} 0 & B_{22} \\ B_{22}^{\mathsf{H}} & 0 \end{pmatrix} \begin{pmatrix} U_{21} \\ V_{21} \end{pmatrix} + \begin{pmatrix} U_{21} \\ V_{21} \end{pmatrix} \Sigma_{11} = \begin{pmatrix} B_{21}V_{11} \\ B_{12}^{\mathsf{H}}U_{11} \end{pmatrix}. \tag{19}$$

Firstly, we bound the first term in the left-hand side of Eq. (19) from above as follows:

$$\begin{aligned} \left\| \begin{pmatrix} 0 & B_{22} \\ B_{22}^{\mathsf{H}} & 0 \end{pmatrix} \begin{pmatrix} U_{21} \\ V_{21} \end{pmatrix} \right\|_{\mathsf{F}} &\leq \left\| \begin{pmatrix} 0 & B_{22} \\ B_{22}^{\mathsf{H}} & 0 \end{pmatrix} \right\|_2 \left\| \begin{pmatrix} U_{21} \\ V_{21} \end{pmatrix} \right\|_{\mathsf{F}} \\ &= \sigma_{\max}(B_{22}) \left\| \begin{pmatrix} U_{21} \\ V_{21} \end{pmatrix} \right\|_{\mathsf{F}}. \end{aligned} \tag{20}$$

Secondly, we bound the norm of the second term $\|(U_{21}^{\mathsf{T}}, V_{21}^{\mathsf{T}})^{\mathsf{T}}\Sigma_{11}\|_{\mathsf{F}}$ from below. Since all singular values of B_{11} are larger than those of B_{22} and the diagonal elements of Σ are ordered non-increasingly, we can apply Corollary 1 to $\mathrm{diag}(B_{11}, B_{22})$ and Σ to show that all singular values of Σ_{11} are within a distance of ω from the corresponding singular values of B_{11}. Hence, using the relation $\sigma_{\min}(B_{11}) = \sigma_{\max}(B_{22}) + \eta$ from the assumption,

$$\sigma_{\min}(\Sigma_{11}) \geq \sigma_{\min}(B_{11}) - \omega = \sigma_{\max}(B_{22}) + \eta - \omega$$

and

$$\|\Sigma_{11}^{-1}\|_2 = (\sigma_{\min}(\Sigma_{11}))^{-1} \leq (\sigma_{\max}(B_{22}) + \eta - \omega)^{-1}.$$

Thus, it follows that

$$\begin{aligned}\left\|\begin{pmatrix} U_{21} \\ V_{21}\end{pmatrix}\right\|_{\mathsf{F}} &\leq \left\|\begin{pmatrix} U_{21} \\ V_{21}\end{pmatrix}\Sigma_{11}\right\|_{\mathsf{F}} \|\Sigma_{11}^{-1}\|_2 \\ &\leq (\sigma_{\max}(B_{22})+\eta-\omega)^{-1}\left\|\begin{pmatrix} U_{21} \\ V_{21}\end{pmatrix}\Sigma_{11}\right\|_{\mathsf{F}},\end{aligned}$$

which leads to

$$\left\|\begin{pmatrix} U_{21} \\ V_{21}\end{pmatrix}\Sigma_{11}\right\|_{\mathsf{F}} \geq (\sigma_{\max}(B_{22})+\eta-\omega)\left\|\begin{pmatrix} U_{21} \\ V_{21}\end{pmatrix}\right\|_{\mathsf{F}}. \tag{21}$$

Thirdly, the right-hand side of Eq. (19) can be bounded as follows. To begin,

$$\begin{aligned}\|(V_{11}^T, U_{11}^T)^T\|_2 &= \max_{\|\mathbf{x}\|=1}\|(V_{11}^T, U_{11}^T)^T\mathbf{x}\|_2 = \max_{\|\mathbf{x}\|=1}\sqrt{\|V_{11}\mathbf{x}\|_2^2+\|U_{11}\mathbf{x}\|_2^2} \\ &\leq \sqrt{\max_{\|\mathbf{x}\|=1}\|V_{11}\mathbf{x}\|_2^2+\max_{\|\mathbf{x}\|=1}\|U_{11}\mathbf{x}\|_2^2} = \sqrt{\|V_{11}\|_2^2+\|U_{11}\|_2^2} \\ &\leq \sqrt{1+1}=\sqrt{2},\end{aligned}$$

so that

$$\begin{aligned}\left\|\begin{pmatrix} B_{21}V_{11} \\ B_{12}^{\mathsf{H}}U_{11}\end{pmatrix}\right\|_{\mathsf{F}} &= \left\|\begin{pmatrix} B_{21} & 0 \\ 0 & B_{12}^{\mathsf{H}}\end{pmatrix}\begin{pmatrix} V_{11} \\ U_{11}\end{pmatrix}\right\|_{\mathsf{F}} \\ &\leq \left\|\begin{pmatrix} B_{21} & 0 \\ 0 & B_{12}^{\mathsf{H}}\end{pmatrix}\right\|_{\mathsf{F}}\left\|\begin{pmatrix} V_{11} \\ U_{11}\end{pmatrix}\right\|_2 \leq \sqrt{2}\,\omega. \end{aligned}\tag{22}$$

Finally, using Eqs. (19), (20), (21), (22) and the lower bound $\|C-D\|_{\mathsf{F}} \geq \|C\|_{\mathsf{F}} - \|D\|_{\mathsf{F}}$ for any two matrices $C,\ D$ of the same size, one gets

$$\begin{aligned}\sqrt{2}\,\omega &\geq \left\|\begin{pmatrix} B_{21}V_{11} \\ B_{12}^{\mathsf{H}}U_{11}\end{pmatrix}\right\|_{\mathsf{F}} \\ &\geq \left\|\begin{pmatrix} U_{21} \\ V_{21}\end{pmatrix}\Sigma_{11}\right\|_{\mathsf{F}} - \left\|\begin{pmatrix} 0 & B_{22} \\ B_{22}^{\mathsf{H}} & 0\end{pmatrix}\begin{pmatrix} U_{21} \\ V_{21}\end{pmatrix}\right\|_{\mathsf{F}} \\ &\geq (\eta-\omega)\left\|\begin{pmatrix} U_{21} \\ V_{21}\end{pmatrix}\right\|_{\mathsf{F}},\end{aligned}$$

which proves the lemma. □

2.2 Convergence of diagonal elements of $A^{(k)}$

In this subsection, we discuss the convergence of the diagonal elements of $A^{(k)}$. Let us write the singular values of A as $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_n > 0$, and let $\Sigma = \mathrm{diag}(\sigma_1, \sigma_2, \ldots, \sigma_n)$. Now, consider the partition of matrix Σ into a $w \times w$ block structure conformably with $A^{(0)}$. At this point, let us formulate following assumptions.

A1 The partition of the initial matrix $A^{(0)}$ into a $w \times w$ block structure is such that each multiple singular value and each cluster of singular values is confined to one diagonal block of Σ. Let σ_{i_r} be the bottom-right singular value in the rth diagonal block of Σ, $1 \le r \le w-1$. Define the global constant δ as

$$\delta \equiv \min_{1\le r\le w-1} (\sigma_{i_r} - \sigma_{i_r+1}),$$

where σ_{i_r+1} is the top-left singular value in the next diagonal block. Consequently, if σ_i and σ_j belong to different diagonal blocks, then $|\sigma_i - \sigma_j| \ge \delta$.

A2 Let k_0 be the smallest integer such that $\|\mathrm{off}(A^{(k)})\|_{\mathsf{F}} \le \delta/4$ for $k \ge k_0$. At iteration step k_0, the rows and columns of $A^{(k_0)}$ are permuted so that the diagonal elements of $A^{(k_0)}$ are ordered non-increasingly.

A3 At each iteration step, the matrices of local left and right singular vectors $\tilde{U}^{(k)}$ and $\tilde{V}^{(k)}$, respectively, in Eq. (1) are computed in such a way that the diagonal elements of $\tilde{A}^{(k+1)} = (\tilde{U}^{(k)})^{\mathsf{H}}\tilde{A}^{(k)}\tilde{V}^{(k)}$ in Eq. (1) are ordered non-increasingly.

Note that the global permutation of $A^{(k)}$ in the assumption **A2** is required only once.

The next theorem is devoted to the convergence of diagonal elements of $A^{(k)}$.

Theorem 3 *Under the assumptions* **A1**, **A2** *and* **A3**, *the iterated matrix $A^{(k)}$ converges to Σ as $k \to \infty$.*

Proof: The proof is very similar to that of [17, Thm. 4]. We show by induction that the diagonal elements of $A^{(k)}$ are already anchored to the singular values, i.e., they are ordered non-increasingly for all k, $k \ge k_0$. The statement is true for $k = k_0$ by the assumption **A2**. Let it be true for some $k \ge k_0$. Since the singular values of $A^{(k)}$ are $\sigma_1 \ge \sigma_2 \ge \cdots \ge \sigma_n$, by setting $B = \mathrm{diag}(a_{11}^{(k)}, a_{22}^{(k)}, \ldots, a_{nn}^{(k)})$ and $C = A^{(k)}$ in Corollary 1, we have

$$|a_{ii}^{(k)} - \sigma_i| \le \|\mathrm{off}(A^{(k)})\|_{\mathsf{F}} \le \frac{\delta}{4}, \;\; i = 1, 2, \ldots, n. \tag{23}$$

Let $a_{pp}^{(k)}$ be the bottom-right diagonal element of some diagonal block and $a_{p+1,p+1}^{(k)}$ be the top-left diagonal element of the next diagonal block of $A^{(k)}$. Since $\sigma_p - \sigma_{p+1} \ge \delta$ from the assumption **A1**, we obtain from the induction hypothesis

$$a_{pp}^{(k)} - a_{p+1,p+1}^{(k)} \ge (\sigma_p - \sigma_{p+1}) - |a_{pp}^{(k)} - \sigma_p| - |a_{p+1,p+1}^{(k)} - \sigma_{p+1}| \ge \frac{\delta}{2}. \tag{24}$$

By the transition from $A^{(k)}$ to $A^{(k+1)}$, the only diagonal elements that change are those belonging to $\tilde{A}^{(k)}$ (see Eqs. (1), (2) and (3)). Let the diagonal elements of $\tilde{A}^{(k)}$ and $\tilde{\Sigma}^{(k+1)}$ be denoted by $\{\tilde{a}_{qq}^{(k)}\}_{q=1}^{2\ell}$ and $\{\tilde{a}_{qq}^{(k+1)}\}_{q=1}^{2\ell}$, respectively. To bound the change $|\tilde{a}_{qq}^{(k+1)} - \tilde{a}_{qq}^{(k)}|$, we use Corollary 1 again. Let

$$B = \tilde{A}^{(k)}, \quad C = \begin{pmatrix} A_{X_kX_k}^{(k)} & O \\ O & A_{Y_kY_k}^{(k)} \end{pmatrix},$$

where $\tilde{A}^{(k)}$ is defined in Eq. (3). Since $\tilde{A}^{(k)}$ and $\tilde{\Sigma}^{(k+1)}$ are connected by the local SVD (see Eqs. (1) and (3)) and $\tilde{\Sigma}^{(k+1)}$ is diagonal, the singular values of B are $\{\tilde{a}_{qq}^{(k+1)}\}_{q=1}^{2\ell}$. In addition, the singular values of C are $\{\tilde{a}_{qq}^{(k)}\}_{q=1}^{2\ell}$, since the matrix blocks $A_{X_kX_k}^{(k)}$ and $A_{Y_kY_k}^{(k)}$ are diagonal. Moreover, using the induction hypothesis and the assumption **A3**, both sets of these diagonal elements are ordered non-increasingly. Hence, using Corollary 1,

$$\begin{aligned}\sum_{q=1}^{2\ell} |\tilde{a}_{qq}^{(k+1)} - \tilde{a}_{qq}^{(k)}|^2 &\leq \|B - C\|_{\mathsf{F}}^2 \\ &\leq \|A_{X_kY_k}^{(k)}\|_{\mathsf{F}}^2 + \|A_{Y_kX_k}^{(k)}\|_{\mathsf{F}}^2 \\ &\leq \|\mathrm{off}(A^{(k)})\|^2 \leq \left(\frac{\delta}{4}\right)^2 . \end{aligned} \tag{25}$$

Since other elements of $A^{(k)}$ are not changed, we have for all i, $1 \leq i \leq n$,

$$|a_{ii}^{(k+1)} - a_{ii}^{(k)}| \leq \frac{\delta}{4}. \tag{26}$$

The combination of Eqs. (24) and (26) gives the following inequality for the index p defined above:

$$\begin{aligned} a_{pp}^{(k+1)} - a_{p+1,p+1}^{(k+1)} &\geq (a_{pp}^{(k)} - a_{p+1,p+1}^{(k)}) - |a_{pp}^{(k+1)} - a_{pp}^{(k)}| - |a_{p+1,p+1}^{(k+1)} - a_{p+1,p+1}^{(k)}| \\ &\geq \frac{\delta}{2} - \frac{\delta}{4} - \frac{\delta}{4} = 0. \end{aligned}$$

Consequently, for any diagonal block of $A^{(k+1)}$, its bottom-right diagonal element is not smaller than the top-left diagonal element of the next diagonal block (if it exists). Since the diagonal elements within each diagonal block are ordered non-increasingly (see the assumption **A3**), it follows that all diagonal elements of $A^{(k+1)}$ are ordered non-increasingly. This completes the induction step. Consequently, Eq. (23) holds for any $k \geq k_0$. Noting that $\|\mathrm{off}(A)^{(k)}\|_{\mathsf{F}}$ converges to zero by Eq. (7) and using Eq. (23), we get $a_{ii}^{(k)} \to \sigma_i$ as $k \to \infty$ for $i = 1, 2, \ldots, n$, so that $A^{(k)} \to \Sigma$. □

During computation, one can obtain an information about the separation of unknown singular values between two adjacent diagonal blocks as shown in the next lemma.

Lemma 2 *At iteration step k, let $d_1^{(k)} = a_{\tau(1),\tau(1)}^{(k)}, d_2^{(k)} = a_{\tau(2),\tau(2)}^{(k)}, \ldots, d_n^{(k)} = a_{\tau(n),\tau(n)}^{(k)}$ be the diagonal elements of $A^{(k)}$ ordered non-increasingly by using a suitable permutation τ, and $D^{(k)} \equiv \mathrm{diag}(d_1^{(k)}, d_2^{(k)}, \ldots, d_n^{(k)})$. Partition the matrix $D^{(k)}$ into a $w \times w$ block structure conformably with $A^{(0)}$, and let the bottom-right elements of the first $w-1$ diagonal blocks be $d_{i_1}^{(k)}, d_{i_2}^{(k)}, \ldots, d_{i_{w-1}}^{(k)}$. If*

$$d_{i_r}^{(k)} - d_{i_r+1}^{(k)} > 3\,\|\mathrm{off}(A^{(k)})\|_{\mathsf{F}}$$

holds for $r = 1, 2, \ldots, w-1$, then

$$\sigma_{i_r} - \sigma_{i_r+1} > \|\mathrm{off}(A^{(k)})\|_{\mathsf{F}}.$$

Proof: The proof is identical with that of [17, Lemma 2]. □

Note that the sorting of $\{a_{ii}^{(k)}\}_{i=1}^{n}$ is required in Lemma 2, but not a global permutation of $A^{(k)}$.

2.3 Convergence of the columns of $U^{(k)}$ and $V^{(k)}$ corresponding to simple singular values

Starting with Eq. (6), let $\mathbf{u}_i^{(k)}$ and $\mathbf{v}_i^{(k)}$ be the ith column of $U^{(k)}$ and $V^{(k)}$, respectively. As we have shown in Theorem 3, $a_{ii}^{(k)}$ converges to the singular value σ_i as $k \to \infty$ under assumptions **A1**, **A2** and **A3**. In this subsection, we consider the convergence of $\mathbf{u}_i^{(k)}$ and $\mathbf{v}_i^{(k)}$ in the case when σ_i is a simple singular value. Note that other singular values of A can be simple or multiple.

Theorem 4 *Let the assumptions* **A1**, **A2** *and* **A3** *hold. If $\sigma_i > 0$ is a simple singular value of A, then the sequence $\{\mathbf{u}_i^{(k)}\}_{k=1}^{\infty}$ and $\{\mathbf{v}_i^{(k)}\}_{k=1}^{\infty}$ converges to the left singular vector $\mathbf{u}_i$ and right singular vector $\mathbf{v}_i$ of A, respectively, corresponding to σ_i.*

Proof: Let δ_i be the smallest distance from σ_i to other singular values of A and k_1 be the smallest integer such that $\|\mathrm{off}(A^{(k)})\|_{\mathsf{F}} \leq \frac{1}{4}\min\{\delta_i, \delta\}$ for $k \geq k_1$, where δ is defined in the assumption **A1**. In the following, we assume that $k \geq k_1$ and consider the transition from $\mathbf{v}_i^{(k)}$ to $\mathbf{v}_i^{(k+1)}$. As we have shown in the proof of Theorem 3, the diagonal elements of $A^{(k)}$ are always ordered non-increasingly for all k, $k \geq k_1 \geq k_0$.

From Eq. (5), $\mathbf{v}_i^{(k+1)}$ is the ith column of $V^{(k)}\hat{V}^{(k)}$. We consider the case where the column i belongs to a block column with the block index either X_k or Y_k; otherwise, $\mathbf{v}_i^{(k+1)} = \mathbf{v}_i^{(k)}$ since $\hat{V}^{(k)}$ are identical to I_n except for two block columns with block indices X_k and Y_k. Denote the block column of $V^{(k)}$ with the block index X_k and Y_k by $V_{X_k}^{(k)}$ and $V_{Y_k}^{(k)}$, respectively, and the local column index of $\mathbf{v}_i^{(k)}$ within the $n \times (2\ell)$ matrix $\begin{pmatrix} V_{X_k}^{(k)} & V_{Y_k}^{(k)} \end{pmatrix}$ by q. Then

$$\mathbf{v}_i^{(k)} = \begin{pmatrix} V_{X_k}^{(k)} & V_{Y_k}^{(k)} \end{pmatrix} \tilde{\mathbf{e}}_q, \quad \mathbf{v}_i^{(k+1)} = \begin{pmatrix} V_{X_k}^{(k)} & V_{Y_k}^{(k)} \end{pmatrix} \tilde{\mathbf{v}}_q^{(k)},$$

where $\mathbf{e}_q$ and $\tilde{\mathbf{v}}_q^{(k)}$ are the qth columns of $I_{2\ell}$ and $\tilde{V}^{(k)}$, respectively. By noting that the matrix $\begin{pmatrix} V_{X_k}^{(k)} & V_{Y_k}^{(k)} \end{pmatrix}$ has orthonormal columns, one gets

$$\|\mathbf{v}_i^{(k+1)} - \mathbf{v}_i^{(k)}\| = \left\| \begin{pmatrix} V_{X_k}^{(k)} & V_{Y_k}^{(k)} \end{pmatrix} (\tilde{\mathbf{v}}_q^{(k)} - \mathbf{e}_q) \right\| = \|\tilde{\mathbf{v}}_q^{(k)} - \mathbf{e}_q\|. \tag{27}$$

To bound the right-hand side of Eq. (27), we use Theorem 2 and Corollary 2. By putting $B = \tilde{A}^{(k)}$ and $\mathbf{x} = \mathbf{y} = \mathbf{e}_q$ in Theorem 2, we have

$$\begin{aligned} \varrho &= \mathbf{e}_q^{\mathsf{H}} B \mathbf{e}_q = \tilde{a}_{qq}^{(k)} = a_{ii}^{(k)}, \quad \varrho \in \mathbb{R},\ \varrho \geq 0, \\ \mathbf{r}(\mathbf{x},\mathbf{y}) &= B\mathbf{y} - \varrho\mathbf{x} = \tilde{\mathbf{a}}_{\star q}^{(k)} - \tilde{a}_{qq}^{(k)}\mathbf{e}_q, \\ \mathbf{s}(\mathbf{x},\mathbf{y}) &= B^{\mathsf{H}}\mathbf{x} - \varrho\mathbf{y} = \left(\tilde{\mathbf{a}}_{q\star}^{(k)}\right)^{\mathsf{H}} - \tilde{a}_{qq}^{(k)}\mathbf{e}_q, \end{aligned}$$

where $\tilde{\mathbf{a}}_{\star q}^{(k)}$and $\tilde{\mathbf{a}}_{q\star}^{(k)}$ is the qth column and row of $\tilde{A}^{(k)}$, respectively. Hence, by noting that $\tilde{a}_{qq}^{(k)}$

is real (and nonnegative) and using Eq. (8),

$$
\begin{aligned}
\|\mathbf{r}(\mathbf{x},\mathbf{y})\| = \left(\sum_{j=1,j\neq q}^{2\ell}\left|\tilde{a}_{jq}^{(k)}\right|^2\right)^{\frac{1}{2}} &\le \|\mathrm{off}(\tilde{A}^{(k)})\|_{\mathsf{F}} \le \|\mathrm{off}(A^{(k)})\|_{\mathsf{F}} \\
&\le \sqrt{S(A)\,\alpha^k}, \\
\|\mathbf{s}(\mathbf{x},\mathbf{y})\| = \left(\sum_{j=1,j\neq q}^{2\ell}\left|\tilde{a}_{qj}^{(k)}\right|^2\right)^{\frac{1}{2}} &\le \|\mathrm{off}(\tilde{A}^{(k)})\|_{\mathsf{F}} \le \|\mathrm{off}(A^{(k)})\|_{\mathsf{F}} \\
&\le \sqrt{S(A)\,\alpha^k}.
\end{aligned}
$$

Next we bound $\mathrm{gap}(\varrho)$ (see Theorem 2) from below. Using the same reasoning as in [17, Eq. (16)], we obtain

$$|\tilde{a}_{qq}^{(k+1)} - \tilde{a}_{qq}^{(k)}| = |a_{ii}^{(k+1)} - a_{ii}^{(k)}| \le \|\mathrm{off}(A^{(k)})\|_{\mathsf{F}} \le \frac{\delta_i}{4}. \tag{28}$$

Moreover, it follows from Corollary 1 that

$$|\tilde{a}_{qq}^{(k)} - \sigma_i| = |a_{ii}^{(k)} - \sigma_i| \le \frac{\delta_i}{4}.$$

Now we consider another diagonal element $\tilde{a}_{rr}^{(k+1)}$ of $\tilde{A}^{(k+1)}$, where $r \neq q$. Let the global index corresponding to r be s (i.e., $\tilde{a}_{rr}^{(k+1)} = a_{ss}^{(k+1)}$). Using Corollary 1 again gives

$$|\tilde{a}_{rr}^{(k+1)} - \sigma_s| = |a_{ss}^{(k+1)} - \sigma_s| \le \frac{\delta_i}{4},$$

so that

$$|\tilde{a}_{rr}^{(k+1)} - \tilde{a}_{qq}^{(k)}| \ge |\sigma_i - \sigma_s| - |\tilde{a}_{rr}^{(k+1)} - \sigma_s| - |\tilde{a}_{qq}^{(k)} - \sigma_i| \ge \frac{\delta_i}{2}. \tag{29}$$

Eqs. (28) and (29) show that $\tilde{a}_{qq}^{(k+1)} = a_{ii}^{(k+1)}$ is the singular value of $\tilde{A}^{(k)}$ closest to $\varrho = \tilde{a}_{qq}^{(k)}$, and all other singular values are separated from $\tilde{a}_{qq}^{(k)}$ by at least $\delta_i/2$. Thus, $\mathrm{gap}(\varrho) \ge \delta_i/2$. The right singular vector of $\tilde{A}^{(k)}$ corresponding to the singular value $\tilde{a}_{qq}^{(k+1)}$ is $\tilde{\mathbf{v}}_q^{(k)}$. Recall that we have chosen the phase factor of $\tilde{\mathbf{v}}_q^{(k)}$ so that its qth element is real and nonnegative (see Eq. (4) in subsection 2.1). Hence, the inner product $(\tilde{\mathbf{v}}_q^{(k)})^{\mathsf{H}}\,\mathbf{e}_q$ is real and nonnegative, and the angle $\theta = \angle(\mathbf{e}_q, \tilde{\mathbf{v}}_q^{(k)})$ is well defined. In contrast, the inner product $(\tilde{\mathbf{u}}_q^{(k)})^{\mathsf{H}}\,\mathbf{e}_q \in \mathbb{C}$ in general. This corresponds to the first "mixed" case that was analyzed in Corollary 2 (see subsection 2.1). Then, applying the bound in Eq. (13),

$$|\sin\theta| \le \frac{\sqrt{\|\mathbf{r}(\mathbf{x},\mathbf{y})\|^2 + \|\mathbf{s}(\mathbf{x},\mathbf{y})\|^2}}{\mathrm{gap}(\varrho)} \le \frac{\sqrt{8S(A)\,\alpha^k}}{\delta_i}.$$

Note that $\cos\theta = (\tilde{\mathbf{v}}_q^{(k)})^{\mathsf{H}}\mathbf{e}_q = \mathbf{e}_q^{\mathsf{H}}\,\tilde{\mathbf{v}}_q^{(k)} = \tilde{v}_{qq}^{(k)} \ge 0$. Inserting these results into Eq. (27) gives

$$
\begin{aligned}
\|\mathbf{v}_i^{(k+1)} - \mathbf{v}_i^{(k)}\|^2 &= \|\tilde{\mathbf{v}}_q^{(k)} - \tilde{\mathbf{e}}_q\|^2 \\
&= \|\tilde{\mathbf{v}}_q^{(k)}\|^2 - \left(\tilde{\mathbf{v}}_q^{(k)}\right)^{\mathsf{H}}\mathbf{e}_q - \mathbf{e}_q^{\mathsf{H}}\,\tilde{\mathbf{v}}_q^{(k)} + \|\mathbf{e}_q\|^2 \\
&= 1 - 2\cos\theta + 1 \\
&\le 2(1-\cos\theta)(1+\cos\theta) \\
&= 2\sin^2\theta \le \frac{16\,S(A)\,\alpha^k}{\delta_i^2},
\end{aligned}
$$

where, in the first inequality, we have used $1 \leq 1 + \cos\theta$. Then,

$$\begin{aligned}\|\mathbf{v}_i^{(k+m)} - \mathbf{v}_i^{(k)}\| &\leq \sum_{j=k}^{k+m-1} \|\mathbf{v}_i^{(j+1)} - \mathbf{v}_i^{(j)}\| \leq \sum_{j=k}^{k+m-1} \frac{4\sqrt{S(A)\,\alpha^j}}{\delta_i} \\ &< \frac{4\sqrt{S(A)\,\alpha^k}}{\delta_i(1-\sqrt{\alpha})}. \end{aligned} \tag{30}$$

Hence, $\{\mathbf{v}_i^{(k)}\}_{k=k_1}^{\infty}$ is the Cauchy sequence and therefore converges to a constant vector $\mathbf{v}_i$ as $k \to \infty$ with $\|\mathbf{v}_i\| = \lim_{k\to\infty} \|\mathbf{v}_i^{(k)}\| = 1$.

Next, we prove the convergence of the sequence $\{\mathbf{u}_i^{(k)}\}_{k=k_1}^{\infty}$. From Eq. (6) and the unitarity of $V^{(k+1)}$ and $U^{(k+1)}$, we have $A^{\mathsf{H}}U^{(k+1)} = V^{(k+1)}\left(A^{(k+1)}\right)^{\mathsf{H}}$. Hence, for the ith column with $a_{ii}^{(k+1)} \in \mathbb{R}$, $a_{ii}^{(k+1)} > 0$,

$$A^{\mathsf{H}}\mathbf{u}_i^{(k+1)} = a_{ii}^{(k+1)}\mathbf{v}_i^{(k+1)} + \sum_{j=1, j\neq i}^{n} \bar{a}_{ij}^{(k+1)}\mathbf{v}_j^{(k+1)}. \tag{31}$$

On the right-hand side of Eq. (31), $\lim_{k\to\infty} a_{ii}^{(k+1)} = \sigma_i > 0$ from Theorem 3, $\lim_{k\to\infty} \mathbf{v}_i^{(k+1)} = \mathbf{v}_i$, and

$$\left\| \sum_{j=1, j\neq i}^{n} \bar{a}_{ij}^{(k+1)}\mathbf{v}_j^{(k+1)} \right\|^2 = \sum_{j=1, j\neq i}^{n} \left| a_{ij}^{(k+1)} \right|^2.$$

Since according to Theorem 3

$$\lim_{k\to\infty} \left| a_{ij}^{(k+1)} \right|^2 = 0, \quad \forall i, j,\ 1 \leq i, j \leq n,\ j \neq i,$$

one has

$$\lim_{k\to\infty} \left\| \sum_{j=1, j\neq i}^{n} \bar{a}_{ij}^{(k+1)}\mathbf{v}_j^{(k+1)} \right\| = 0,$$

so that

$$\lim_{k\to\infty} \sum_{j=1, j\neq i}^{n} \bar{a}_{ij}^{(k+1)}\mathbf{v}_j^{(k+1)} = \mathbf{0}.$$

In summary, there must exist $\lim_{k\to\infty} A^{\mathsf{H}}\mathbf{u}_i^{(k+1)}$ of the left-hand side of Eq. (31). Since A^{H} is regular, it is a linear, continuous and one-to-one mapping from $\mathbb{C}^n$ onto $\mathbb{C}^n$. Consequently, the sequence $\{\mathbf{u}_i^{(k)}\}_{k=1}^{\infty}$ converges to a constant vector $\mathbf{u}_i$ with $\|\mathbf{u}_i\| = \lim_{k\to\infty} \|\mathbf{u}_i^{(k)}\| = 1$, and

$$A^H\mathbf{u}_i = \sigma_i\mathbf{v}_i. \tag{32}$$

On the other hand, using Eq. (6) again,

$$A\mathbf{v}_i^{(k+1)} = a_{ii}^{(k+1)}\mathbf{u}_i^{(k+1)} + \sum_{j=1, j\neq i}^{n} a_{ji}^{(k+1)}\mathbf{u}_j^{(k+1)},$$

and repeating the above arguments, one gets after taking the limit $k \to \infty$:

$$A\mathbf{v}_i = \sigma_i\mathbf{u}_i. \tag{33}$$

Eqs. (32) and (33) show, by definition, that (u_i, σ_i, v_i) is indeed the ith singular triplet of A. □

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