Scaled Iterates by Kogbetliantz Method

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Abstract. Scaled iterates associated with the serial Kogbetliantz method for computing the singular value decomposition (SVD) of complex triangular matrices are considered. They are defined by $B_S^{(k)} = |\operatorname{diag}(B^{(k)})|^{-1/2} B^{(k)} |\operatorname{diag}(B^{(k)})|^{-1/2}$, where $B^{(k)}$ are matrices generated by the method. Sharp estimates are derived for the Frobenius norm of the off-diagonal part of $B_S^{(k)}$, in the case of simple singular values. This norm represents a good measure of advancement of the algorithm. The obtained estimates can be used in connection with the quadratic convergence of the algorithm.

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1. Introduction

Kogbetliantz method is a known two-sided SVD Jacobi method for square matrices. Since its discovery [16, 17], the method has been thoroughly studied, especially its global convergence [10], its quadratic convergence [22, 11, 3], and its implementation details [2, 18, 4, 5, 7]. Later, it was found out that the method becomes more simple and efficient if it is applied to a triangular initial matrix under the row-cyclic or column-cyclic pivot strategy (see [15]). In that case, the method exhibits a behavior very similar to the known Jacobi method for symmetric/Hermitian matrices (see [15, 12, 9, 13]). The starting triangular matrix is obtained by applying the QR factorization once or twice (cf. [8]).

Although it has not been proved yet, numerical tests lead to presumption, that on triangular matrices obtained by the QR factorization with column pivoting, the serial Kogbetliantz method computes the singular values and vectors with high relative accuracy.

In the recent paper [21] (see also Theorem 1 here) it has been shown that a proper measure for the relative distance between diagonal elements and the corresponding singular values is the norm of the off-diagonal part (the so-called off-norm) of the scaled matrix, divided by the minimum relative gap in the set of singular values. Since this relative gap depends only on the initial matrix, one is forced to monitor the off-norm of the scaled iterates.

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The same conclusion holds for the Hermitian Jacobi method when applied to positive definite matrices (see [6]). The same will hold (cf. [1, 14]) if the initial matrix is scaled diagonally dominant indefinite Hermitian matrix. In these cases, however, sharp quadratic convergence bounds of scaled iterates have already been proved in [19] and [20]. These results have nice applications in connection with the stopping criteria of one- and two-sided Hermitian Jacobi methods.

In this paper we estimate the off-norms of scaled iterates for the complex Kogbetliantz method under the column-cyclic pivot strategy, in the case of simple singular values. Although elementary, some proofs presented here are quite long and complex. The estimates presented are generalizations of those from [20]. As an application, we sketch how the new estimates can be used in the quadratic convergence proof of the serial Kogbetliantz method. We believe that another application lies in the accuracy consideration of the method.

In the same fashion as the estimates from [14] have been used in [20], here the estimates from [21] are used. The role of the minimum absolute gap in the classical result [25, 13], is replaced here by the minimum relative gap. Therefore, the obtained results are especially well suited for the case when singular values cluster around the origin.

Note that the proof of the quadratic convergence of scaled iterates by the Hermitian Jacobi method from [20] is much more complicated than the already complicated proof for the non-scaled iterates from [13, 23]. A similar, although somewhat more complex situation is present here, so acquaintance with the proofs from [20] could help in understanding this paper.

The paper is organized as follows. In Section 2 we present recent results on scaled diagonally dominant triangular matrices, based on the relative gaps in the set of singular values. In Section 3 we briefly describe the complex Kogbetliantz method. In Section 4 we prove some general, and in Section 5 some asymptotic estimates for scaled iterates. As an application, in the last section we formulate asymptotic assumptions that are needed for the quadratic convergence of scaled iterates in the case of simple singular values. We also briefly sketch the quadratic convergence proof.

2. Notation and auxiliaries

First we introduce notation. By $\mathbb{C}^{n\times n}$ we denote the set of complex matrices of order n. For every $X \in \mathbb{C}^{n\times n}$, $\operatorname{diag}(X) = \operatorname{diag}(x_{11}, \ldots, x_{nn})$ is the diagonal part, and

$$\Omega(X) = X - \operatorname{diag}(X)$$

is the off-diagonal part of $X = (x_{ij})$. The *i*-th row of $\Omega(X)$ is denoted by $\tau_i(X)$ (cf. [14]), i.e.,

$$\tau_i(X) = [x_{i1} \dots x_{i,i-1} \ 0 \ x_{i,i+1} \dots x_{in}]. \tag{1}$$

If X has invertible diag(X), then

$$X_S = |\operatorname{diag}(X)|^{-1/2} X |\operatorname{diag}(X)|^{-1/2}$$
(2)

is regarded as the scaled matrix X. Note that the scaled matrix X_S has diagonal elements of unit modulus.

If $\|\Omega(X_S)\| \le \alpha < 1$, then X is an α -scaled diagonally dominant (α -s.d.d.) matrix with respect to a norm $\|\cdot\|$ (see [1]). The spectral and the Frobenius norm of X will be denoted by $\|X\|_2$ and $\|X\|$, respectively.

Let us introduce yet the relative gap function rg of two real arguments (see [14]),

$$rg(a,b) = \begin{cases} \frac{|a-b|}{|a|+|b|}, & \text{if } |a|+|b| > 0, \\ 0, & \text{if } a=b=0. \end{cases}$$
 (3)

Let $B \in \mathbb{C}^{n \times n}$ have simple singular values

$$\sigma_1 > \sigma_2 > \sigma_3 > \dots > \sigma_n. \tag{4}$$

By using (3) and (4), we define the relative gaps in the set of singular values of B,

$$\theta_i = \min_{\substack{1 \le j \le n \\ j \ne i}} \operatorname{rg}(\sigma_i, \sigma_j), \quad 1 \le i \le n,$$
(5)

and the minimum relative gap

$$\theta = \min_{1 \le i \le n} \theta_i. \tag{6}$$

Note that $\theta_i < 1$ for all $1 \le i \le n$.

The structure of an α -s.d.d. matrix is given in [21]. In this paper we consider only triangular and essentially triangular α -s.d.d. matrices B with simple singular values (see Section 3). For such matrices $b_{ij} \cdot b_{ji} = 0$ holds for $i \neq j$, and the result from [21, Corollary 6] takes the following form.

Theorem 1. Let $B \in \mathbb{C}^{n \times n}$ be an essentially triangular matrix with positive diagonal, satisfying

$$b_{11} > b_{22} > \dots > b_{nn} \tag{7}$$

and

$$\|\Omega(B_S)\|_2 < \frac{\theta}{3},\tag{8}$$

where B_S and θ are defined by (2) and (6), respectively. If the singular values of B are simple, then

(i)
$$\left| 1 - \frac{\sigma_i}{b_{ii}} \right| \le \frac{2}{\theta_i} (\|\tau_i(B_S)\|^2 + \|\tau_i(B_S^*)\|^2), \quad 1 \le i \le n,$$

(ii)
$$\sum_{i=1}^{n} \left| 1 - \frac{\sigma_i}{b_{ii}} \right|^2 \le \frac{8}{\theta^2} \|\Omega(B_S)\|^4,$$

where $\tau_i(\cdot)$ and θ_i are defined by (1) and (5), respectively.

 $^{^{1}\}mathrm{We}$ use only the symmetric scaling.

If diag(B) is not positive definite, every appearance of diagonal elements of B (in the assumption (7), and in the assertions (i) and (ii)) should be replaced by their moduli. Theorem 1 is used in the asymptotic estimates for scaled iterates by the Kogbetliantz method.

3. Kogbetliantz method

Here we give a short description of the Kogbetliantz method for computing the singular value decomposition of triangular matrices (SVDT). Let $B = (b_{lm})$ be a complex triangular matrix of order n, with positive diagonal elements satisfying the assumption (7). Note that (7) naturally results after applying the QR factorization with column pivoting. The Kogbetliantz method for complex triangular matrices has a nice property of maintaining the reality (positivity) of the initially real (positive) diagonal elements. Since real, or even better, positive diagonal elements, make the algorithm simpler, we assume the initial matrix B has a positive diagonal which satisfies (7).

Note also that for any square complex matrix the condition (7) can be achieved by considering the matrix $P^*\Phi^*BP$, where $\Phi = \operatorname{diag}(e^{i\operatorname{arg}(b_{11})},\dots,e^{i\operatorname{arg}(b_{nn})})$, and P is a suitably chosen permutation matrix. The matrices B and $P^*\Phi^*BP$ have the same singular values, while the singular vectors are simply related. If B is a triangular matrix for which $|b_{11}| > \dots > |b_{nn}|$ holds, then $P = I_n$.

Starting from a triangular matrix B, the Kogbetliantz method generates a sequence of matrices $B^{(k)} = (b_{lm}^{(k)}), k \ge 0$, by the rule

$$B^{(0)} = B, \quad B^{(k+1)} = (U^{(k)})^* B^{(k)} V^{(k)}, \quad k \ge 0,$$
 (9)

where $U^{(k)}$ and $V^{(k)}$ are unitary plane matrices whose essential four elements are

$$\begin{split} & \left(U^{(k)}\right)_{ii} = \left(U^{(k)}\right)_{jj} = \cos\varphi^{(k)} & \left(U^{(k)}\right)_{ij} = -\left(\overline{U^{(k)}}\right)_{ji} = e^{\imath\omega_k}\sin\varphi^{(k)} \\ & \left(V^{(k)}\right)_{ii} = \left(V^{(k)}\right)_{jj} = \cos\psi^{(k)} & \left(V^{(k)}\right)_{ij} = -\left(\overline{V^{(k)}}\right)_{ji} = e^{\imath\vartheta_k}\sin\psi^{(k)}. \end{split}$$

For the other elements, we have $(U^{(k)})_{lm} = (V^{(k)})_{lm} = \delta_{lm}$, $\{l,m\} \cap \{i,j\} = \emptyset$. Here, i is the imaginary unit, \bar{z} is the complex conjugate of z, and δ_{lm} is the Kronecker's delta. The 2×2 matrices

$$\begin{bmatrix} b_{ii}^{(k)} & b_{ij}^{(k)} \\ b_{ji}^{(k)} & b_{jj}^{(k)} \end{bmatrix}, \quad \begin{bmatrix} (U^{(k)})_{ii} & (U^{(k)})_{ij} \\ (U^{(k)})_{ji} & (U^{(k)})_{jj} \end{bmatrix}, \quad \begin{bmatrix} (V^{(k)})_{ii} & (V^{(k)})_{ij} \\ (V^{(k)})_{ji} & (V^{(k)})_{jj} \end{bmatrix},$$

are called the *pivot submatrices* of $B^{(k)}$, $U^{(k)}$, $V^{(k)}$, respectively. The pair of indices (i,j)=(i(k),j(k)) is called the *pivot pair* and $b^{(k)}_{ij}$ is the *pivot element*. The relation (9) defines the k-th step or the k-th iteration of the method. In the sequel, i and j will be reserved for pivot indices.

For $b_{ij}^{(k)} \neq 0$, the angles $\varphi^{(k)}$, $\psi^{(k)}$, ω_k and ϑ_k are determined by the requirement

$$b_{ij}^{(k+1)} = b_{ji}^{(k+1)} = 0, (10)$$

which ensures that

$$\|\Omega(B^{(k+1)})\|^2 = \|\Omega(B^{(k)})\|^2 - |b_{ij}^{(k)}|^2, \quad k \ge 0.$$
(11)

The requirement (10) yields several sets of formulas for required angles, depending on whether $U^{(k)}$ or $V^{(k)}$ is calculated first (see [10, 24, 4, 12, 13]). Here we consider only the serial, that is, the column- and the row-cyclic pivot strategies. In the first case, the pivot pair cycles through the sequence $(1,2),(1,3),(2,3),\ldots,(1,n),\ldots,(n-1,n)$. In the second case, the sequence is $(1,2),\ldots,(1,n),(2,3),\ldots,(2,n),\ldots,(n-1,n)$.

Serial Kogbetliantz methods do not essentially ruin the triangular form. If B is upper triangular, then within an odd (even) cycle, the nontrivial off-diagonal elements push downwards (upwards), so that after each odd (even) sweep the current matrix is lower (upper) triangular. A similar situation is when B is lower triangular. Within every cycle, each current matrix is permutationally similar to a matrix in triangular form (PST), hence it is essentially triangular (see [15]). Therefore, the whole process can be performed on an upper triangular array (see [12, 13]). At step k, we can associate the upper triangular matrix $G^{(k)} = (g_{lm}^{(k)})$ with the content of that array. Then, we have

$$G^{(k)} + (G^{(k)})^T = B^{(k)} + (B^{(k)})^T, \quad k \ge 0.$$
 (12)

In the following we assume positive diagonal elements. We shall express the angle formulas in terms of the elements of $G^{(k)}$. If the right-hand transformation $V^{(k)}$ is computed first, then (10) implies

$$\begin{split} e^{i\vartheta_k} \tan 2\psi^{(k)} &= \frac{2g_{ii}^{(k)}g_{ij}^{(k)}}{\left(g_{jj}^{(k)}\right)^2 - \left(g_{ii}^{(k)}\right)^2 + \left|g_{ij}^{(k)}\right|^2}, \\ e^{i\omega_k} \tan \varphi^{(k)} &= e^{i\vartheta_k} \frac{\left|g_{ij}^{(k)}\right| + g_{ii}^{(k)} \tan \psi^{(k)}}{g_{ij}^{(k)}} = \frac{g_{jj}^{(k)}e^{i\vartheta_k} \tan \psi^{(k)}}{g_{ii}^{(k)} - \left|g_{ij}^{(k)}\right| \tan \psi^{(k)}}. \end{split}$$

Hence, we obtain the following angle formulas (see [24, 12, 13]) for the first sweep:

$$e^{i\vartheta_k} = \frac{g_{ij}^{(k)}}{|g_{ij}^{(k)}|}, \quad \text{i.e.,} \quad \vartheta_k = \arg\left(g_{ij}^{(k)}\right), \tag{13}$$

$$\tan 2\psi^{(k)} = \frac{2g_{ii}^{(k)}|g_{ij}^{(k)}|}{(g_{ij}^{(k)})^2 - (g_{ii}^{(k)})^2 + |g_{ij}^{(k)}|^2}, \quad \psi^{(k)} \in \left[-\frac{\pi}{4}, \frac{\pi}{4} \right], \tag{14}$$

$$z_k = \frac{g_{ij}^{(k)} + g_{ii}^{(k)} e^{i\vartheta_k} \tan \psi^{(k)}}{g_{jj}^{(k)}} = e^{i\vartheta_k} \frac{\left| g_{ij}^{(k)} \right| + g_{ii}^{(k)} \tan \psi^{(k)}}{g_{jj}^{(k)}}$$

$$= \frac{g_{jj}^{(k)} e^{i\vartheta_k} \tan \psi^{(k)}}{g_{ii}^{(k)} - |g_{ij}^{(k)}| \tan \psi^{(k)}},$$
(15)

$$e^{i\omega_k} = \frac{z_k}{|z_k|}, \quad \text{i.e.,} \quad \omega_k = \arg(z_k),$$
 (16)

$$\tan \varphi^{(k)} = |z_k|, \quad \varphi^{(k)} \in \left[0, \frac{\pi}{2}\right]. \tag{17}$$

Using the notation: $c_{\varphi}^{(k)} = \cos \varphi^{(k)}$, $s_{\varphi}^{(k)} = \sin \varphi^{(k)}$, $c_{\psi}^{(k)} = \cos \psi^{(k)}$, $s_{\psi}^{(k)} = \sin \psi^{(k)}$, the transformation formulas for the elements of $G^{(k)}$ become

$$\begin{split} g_{li}^{(k+1)} &= c_{\varphi}^{(k)} g_{li}^{(k)} - e^{\imath \omega_k} s_{\varphi}^{(k)} g_{lj}^{(k)}} \\ g_{lj}^{(k+1)} &= e^{-\imath \omega_k} s_{\varphi}^{(k)} g_{li}^{(k)} + c_{\varphi}^{(k)} g_{lj}^{(k)}} \\ g_{lj}^{(k+1)} &= c_{\psi}^{(k)} g_{il}^{(k)} - e^{-\imath \vartheta_k} s_{\psi}^{(k)} g_{lj}^{(k)}} \\ g_{lj}^{(k+1)} &= e^{\imath \vartheta_k} s_{\psi}^{(k)} g_{il}^{(k)} + c_{\psi}^{(k)} g_{lj}^{(k)}} \\ g_{lj}^{(k+1)} &= e^{\imath \vartheta_k} s_{\psi}^{(k)} g_{il}^{(k)} + c_{\psi}^{(k)} g_{lj}^{(k)}} \\ g_{il}^{(k+1)} &= c_{\varphi}^{(k)} g_{il}^{(k)} - e^{\imath \omega_k} s_{\varphi}^{(k)} g_{jl}^{(k)}} \\ g_{jl}^{(k+1)} &= e^{-\imath \omega_k} s_{\varphi}^{(k)} g_{il}^{(k)} + c_{\varphi}^{(k)} g_{jl}^{(k)}} \\ g_{ii}^{(k+1)} &= \frac{c_{\varphi}^{(k)}}{c_{\psi}^{(k)}} g_{ii}^{(k)} = \frac{\left|s_{\psi}^{(k)}\right|}{s_{\varphi}^{(k)}} g_{jj}^{(k)} = \frac{c_{\psi}^{(k)}}{c_{\varphi}^{(k)}} g_{ii}^{(k)} - \frac{s_{\psi}^{(k)}}{c_{\varphi}^{(k)}} \left|g_{ij}^{(k)}\right|, \\ g_{ij}^{(k+1)} &= \frac{c_{\psi}^{(k)}}{c_{\varphi}^{(k)}} g_{jj}^{(k)} = \frac{s_{\varphi}^{(k)}}{\left|s_{\psi}^{(k)}\right|} g_{ii}^{(k)} = \frac{c_{\varphi}^{(k)}}{c_{\psi}^{(k)}} g_{jj}^{(k)} + \operatorname{sign}\left(s_{\psi}^{(k)}\right) \frac{s_{\varphi}^{(k)}}{c_{\psi}^{(k)}} \left|g_{ij}^{(k)}\right|, \\ g_{ij}^{(k+1)} &= 0. \end{split}$$

The transformation $G^{(k)} \to G^{(k+1)}$, defined by the relations (13)–(17) and (18) will be called the *Kogbetliantz transformation* or the *Kogbetliantz step* on the associated matrix $G^{(k)}$, with the pivot pair (i,j), or, briefly, the associated Kogbetliantz transformation or step. The algorithm (or the whole process) on matrices $G^{(k)}$ will be called the associated Kogbetliantz algorithm (process).

Starting with an upper triangular B, the relation (18) holds for odd cycles only. For even cycles, the angles interchange their places: $\varphi^{(k)} \leftrightarrow \psi^{(k)}$ and $\omega_k \leftrightarrow \vartheta_k$. We can consider a method in which $U^{(k)}$ and $V^{(k)}$ interchange their places in subsequent cycles, and thus ensure that (18) holds for every cycle². But, in the end, the obtained bounds are symmetric in the arguments $\varphi^{(k)}$ and $\psi^{(k)}$. Therefore, we do not consider the angle formulas for the case when $U^{(k)}$ is calculated first.

Let us now consider the scaled iterates of the matrices $G^{(k)}$,

$$G_S^{(k)} = \left| \operatorname{diag} \left(G^{(k)} \right) \right|^{-1/2} G^{(k)} \left| \operatorname{diag} \left(G^{(k)} \right) \right|^{-1/2}, \quad k \ge 0.$$
 (19)

The matrix $G_S^{(k)}$ is associated with the content of an upper triangular array where

²The interchanges reflect only on singular vector updates.

 $B_S^{(k)}$ is compactly stored in. Next, we define

$$A^{(k)} = \Omega(G_S^{(k)} + (G_S^{(k)})^T) = \Omega(G_S^{(k)}) + \Omega(G_S^{(k)})^T, \quad k \ge 0.$$
 (20)

Note that $A^{(k)} = (a_{lm}^{(k)})$ is a symmetric matrix with zero diagonal, whose off-diagonal elements are given by

$$a_{lm}^{(k)} = a_{ml}^{(k)} = \frac{g_{lm}^{(k)}}{\sqrt{g_{ll}^{(k)}g_{mm}^{(k)}}}, \quad l \neq m, \quad k \ge 0.$$
 (21)

Since each $B_S^{(k)}$ is essentially triangular, the relations (12), (2), (19) and (20) imply

$$A^{(k)} = \Omega(B_S^{(k)}) + \Omega(B_S^{(k)})^T, \quad k \ge 0.$$

Hence

$$a_{lm}^{(k)} = \frac{b_{lm}^{(k)} + b_{ml}^{(k)}}{\sqrt{b_{ll}^{(k)}b_{mm}^{(k)}}}, \quad l \neq m, \quad k \geq 0.$$

The Frobenius norm of $\Omega(G_S^{(k)})$ will be denoted by α_k ,

$$\alpha_k = \|\Omega(G_S^{(k)})\| = \|\Omega(B_S^{(k)})\| = \frac{\sqrt{2}}{2} \|A^{(k)}\|, \quad k \ge 0.$$
 (22)

This paper estimates the changes of α_k within one cycle. To this end, we can presume that k=0. We shall consider both general estimates, and estimates that require α_0 to be small enough.

4. General estimates

Here, we obtain estimates that do not require small α_0 . From (11), we conclude that

$$\left\| \Omega \big(G^{(k+1)} \big) \right\|^2 = \left\| \Omega \big(G^{(k)} \big) \right\|^2 - \left| g_{ij}^{(k)} \right|^2, \quad k \geq 0.$$

This property is not shared by the sequence $\|\Omega(G_S^{(k)})\|^2$, because $G_S^{(k)} \to G_S^{(k+1)}$ is not an orthogonal transformation. Let us consider this transformation more carefully.

Lemma 1. Suppose the sequence $G^{(k)} = (g_{lm}^{(k)})$, $k \geq 0$, is obtained by the associated Kogbetliantz process, and suppose that $G^{(0)}$ has positive diagonal elements. For a fixed k, let us denote $G = (g_{lm}) = G^{(k)}$ and $\widetilde{G} = (\widetilde{g}_{lm}) = G^{(k+1)}$. Thus, \widetilde{G} is obtained from G by a single Kogbetliantz transformation which annihilates the element g_{ij} . Let $A = (a_{lm})$ and $\widetilde{A} = (\widetilde{a}_{lm})$ be defined by

$$A = \Omega(G_S) + \Omega(G_S)^T$$
, $\widetilde{A} = \Omega(\widetilde{G}_S) + \Omega(\widetilde{G}_S)^T$.

If $|a_{ij}| < 1$, then

$$|\tilde{a}_{li}|^2 + |\tilde{a}_{lj}|^2 \le \frac{1 + |a_{ij}|}{1 - |a_{ij}|} (|a_{li}|^2 + |a_{lj}|^2), \quad l \ne i, j.$$

Proof. Note that the diagonal of $G^{(k)}$ remains positive during the process. In the proof we omit the index k. By using (18), for $1 \le l \le i - 1$, we obtain

$$|\tilde{g}_{li}|^2 = c_{\varphi}^2 |g_{li}|^2 + s_{\varphi}^2 |g_{li}|^2 - 2s_{\varphi} c_{\varphi} \operatorname{Re}(e^{i\omega} \bar{g}_{li} g_{li}), \tag{23}$$

$$|\tilde{g}_{lj}|^2 = c_{\varphi}^2 |g_{lj}|^2 + s_{\varphi}^2 |g_{li}|^2 + 2s_{\varphi} c_{\varphi} \operatorname{Re}(e^{\imath \omega} \bar{g}_{li} g_{lj}). \tag{24}$$

Now, by using (21), (23) and (24), we have

$$(|\tilde{a}_{li}|^{2} + |\tilde{a}_{lj}|^{2}) - (|a_{li}|^{2} + |a_{lj}|^{2}) = \left(\frac{|\tilde{g}_{li}|^{2}}{\tilde{g}_{ii}g_{ll}} + \frac{|\tilde{g}_{lj}|^{2}}{\tilde{g}_{jj}g_{ll}}\right) - \left(\frac{|g_{li}|^{2}}{g_{ii}g_{ll}} + \frac{|g_{lj}|^{2}}{g_{jj}g_{ll}}\right)$$

$$= \frac{1}{g_{ll}} \cdot \left(\frac{|\tilde{g}_{li}|^{2}}{\tilde{g}_{ii}} + \frac{|\tilde{g}_{lj}|^{2}}{\tilde{g}_{jj}} - \frac{|g_{li}|^{2}}{g_{ii}} - \frac{|g_{lj}|^{2}}{g_{jj}}\right)$$

$$= \left(\underbrace{\frac{c_{\varphi}^{2}}{\tilde{g}_{ii}} + \frac{s_{\varphi}^{2}}{\tilde{g}_{jj}} - \frac{1}{g_{ii}}}_{\omega_{i\varphi}}\right) \cdot \frac{|g_{li}|^{2}}{g_{ll}} + \left(\underbrace{\frac{c_{\varphi}^{2}}{\tilde{g}_{jj}} + \frac{s_{\varphi}^{2}}{\tilde{g}_{ii}} - \frac{1}{g_{jj}}}_{\omega_{j\varphi}}\right) \cdot \frac{|g_{lj}|^{2}}{g_{ll}}$$

$$+ \underbrace{2s_{\varphi}c_{\varphi} \cdot \left(\frac{1}{\tilde{g}_{jj}} - \frac{1}{\tilde{g}_{ii}}\right)}_{\omega_{i\varphi}} \cdot \underbrace{\frac{\operatorname{Re}(e^{i\omega}\bar{g}_{li}g_{lj})}{g_{ll}}}_{g_{ll}}, \quad 1 \leq l \leq i - 1. \quad (25)$$

The relation (25) also holds for $i+1 \leq l \leq j-1$, provided that c_{φ} , s_{φ} , g_{li} , are replaced by c_{ψ} , s_{ψ} , g_{il} , respectively, and for $j+1 \leq l \leq n$, provided that g_{li} , g_{lj} , are replaced by g_{il} , g_{jl} , respectively. Our next task is to find sharp upper bounds for $\omega_{i\varphi}$, $\omega_{j\varphi}$, $|\omega_{\varphi}|$, $|\omega_{i\psi}|$, $|\omega_{i\psi}|$, $|\omega_{\psi}|$, where the last three terms are defined in the same way as the first three, with φ being replaced by ψ . Although the desired estimates are obtained by using elementary calculus, the way is quite complicated.

In order to simplify the notation, we set

$$a := |a_{ij}| = \frac{|g_{ij}|}{\sqrt{g_{ii}g_{jj}}}.$$

We start with some basic relations between ψ and φ that follow from (17) and (14):

$$\tan \varphi \ge 0, \quad |\tan \psi| \le 1, \tag{26}$$

$$sign(\tan \psi) = sign(\tan 2\psi) = sign(g_{ij}^2 - g_{ij}^2 + |g_{ij}|^2).$$
 (27)

According to (27), we consider two cases: $\tan \psi < 0$, and $\tan \psi \ge 0$. In both cases, $g_{ij} \ne 0$ is presumed, since otherwise all angles are zero, the transformation is skipped,

and the assertion of the lemma holds with equality. This means that to the rest of the proof, both angles φ and ψ are nontrivial.

(a) If $\tan \psi < 0$, then we have $g_{jj}^2 + |g_{ij}|^2 < g_{ii}^2$, hence $g_{jj} < g_{ii}$. From (15) and (17), we obtain

$$\tan \varphi < \frac{g_{jj}}{g_{ii}} |\tan \psi| < |\tan \psi|. \tag{28}$$

Since $g_{jj} \tan \varphi = ||g_{ij}| - g_{ii}|\tan \psi||$, we have

$$|\tan \psi| \le \frac{g_{jj}}{g_{ii}} \tan \varphi + \frac{|g_{ij}|}{g_{ii}} < \tan \varphi + \frac{|g_{ij}|}{g_{ii}} < \tan \varphi + a. \tag{29}$$

- (b) If $\tan \psi > 0$, then $g_{jj}^2 + |g_{ij}|^2 > g_{ii}^2$, and we consider two further subcases.
- (b1) Assume $g_{ii} \geq g_{jj}$. From (15), we have $g_{jj} \tan \varphi = |g_{ij}| + g_{ii} |\tan \psi|$, whence

$$|\tan \psi| = \tan \psi = \frac{g_{jj}}{g_{ii}} \tan \varphi - \frac{|g_{ij}|}{g_{ii}} < \frac{g_{jj}}{g_{ii}} \tan \varphi \le \tan \varphi. \tag{30}$$

Note that a < 1, by assumption. Since, by (26),

$$|g_{ij}| |\tan \psi| \le |g_{ij}| = a \cdot \sqrt{g_{ii}g_{jj}} \le ag_{ii} < g_{ii}, \quad \text{and} \quad \frac{|g_{ij}|}{g_{ii}} = a\sqrt{\frac{g_{jj}}{g_{ii}}} \le a,$$

from the last expression in (15), we obtain

$$\frac{\tan \varphi}{|\tan \psi|} = \frac{\tan \varphi}{\tan \psi} \le \frac{g_{jj}}{g_{ii} - |g_{ij}| \tan \psi} < \frac{g_{jj}}{g_{ii}} \cdot \frac{1}{1 - |g_{ij}|/g_{ii}} \le \frac{1}{1 - |g_{ij}|/g_{ii}}, \quad (31)$$

and

$$\frac{\tan \varphi}{\tan \psi} \le \frac{g_{jj}}{g_{ii}} \cdot \frac{1}{1-a} \le \frac{1}{1-a}.$$
(32)

(b2) Assume $g_{jj} > g_{ii}$. Since

$$|g_{ij}| |\tan \psi| \le \frac{g_{ii}|g_{ij}|^2}{g_{jj}^2 - g_{ii}^2 + |g_{ij}|^2} < g_{ii},$$

the last expression in (15) implies $g_{ii} \tan \varphi - |g_{ij}| \tan \varphi |\tan \psi| = g_{jj} |\tan \psi|$. Hence

$$|\tan \psi| = \tan \psi = \frac{g_{ii}}{g_{jj}} \tan \varphi - \frac{|g_{ij}|}{g_{jj}} \tan \varphi \tan \psi < \frac{g_{ii}}{g_{jj}} \tan \varphi < \tan \varphi.$$
 (33)

In this case we obtain the following estimates for the angle φ ,

$$\tan \varphi = \frac{1}{g_{jj}} (|g_{ij}| + g_{ii} \tan \psi) = a \sqrt{\frac{g_{ii}}{g_{jj}}} + \frac{g_{ii}}{g_{jj}} \tan \psi < a \sqrt{\frac{g_{ii}}{g_{jj}}} + \tan \psi, \tag{34}$$

and

$$\tan \varphi < \sqrt{\frac{g_{ii}}{g_{ij}}} \cdot (a + \tan \psi) < a + \tan \psi. \tag{35}$$

Since $g_{ii} \tan \varphi = g_{jj} \tan \psi + |g_{ij}| \tan \varphi \tan \psi$, by using (35) and (26), we also obtain

$$\frac{\tan \varphi}{\tan \psi} = \frac{g_{jj}}{g_{ii}} + \frac{|g_{ij}|}{g_{ii}} \tan \varphi = \frac{g_{jj}}{g_{ii}} \left(1 + \frac{|g_{ij}|}{g_{jj}} \tan \varphi \right) \le \frac{g_{jj}}{g_{ii}} (1 + a \tan \varphi) \tag{36}$$

$$<\frac{g_{jj}}{g_{ii}}(1+a(\tan\psi+a))<\frac{g_{jj}}{g_{ii}}(1+a(1+a)).$$
 (37)

Now we shall bound $\omega_{i\varphi}$, $\omega_{j\varphi}$, $|\omega_{\varphi}|$, $\omega_{i\psi}$, $|\omega_{j\psi}|$. For each term we have to consider three cases: (a), (b1) and (b2).

Bound for $\omega_{i\varphi}$. From (25) and (18), we obtain

$$\omega_{i\varphi} = \frac{c_{\varphi}^{2}}{g_{jj}|s_{\psi}|/s_{\varphi}} + \frac{s_{\varphi}^{2}}{g_{jj}c_{\psi}/c_{\varphi}} - \frac{1}{g_{ii}} = \frac{1}{g_{ii}} \left[\frac{g_{ii}}{g_{jj}} \left(\frac{s_{\varphi}c_{\varphi}^{2}}{|s_{\psi}|} + \frac{s_{\varphi}^{2}c_{\varphi}}{c_{\psi}} \right) - 1 \right]$$

$$= \frac{1}{g_{ii}} \left[\frac{g_{ii}}{g_{jj}} \cdot \frac{s_{\varphi}c_{\varphi}}{|s_{\psi}|c_{\psi}} \left(c_{\varphi}c_{\psi} + s_{\varphi}|s_{\psi}| \right) - 1 \right]$$

$$= \frac{1}{g_{ii}} \left[\frac{g_{ii}}{g_{jj}} \cdot \frac{s_{\varphi}/c_{\varphi}}{|s_{\psi}|/c_{\psi}} \cdot \frac{1/c_{\psi}^{2}}{1/c_{\varphi}^{2}} \left(c_{\varphi}c_{\psi} + s_{\varphi}|s_{\psi}| \right) - 1 \right]$$

$$= \frac{1}{g_{ii}} \left[\frac{g_{ii}}{g_{jj}} \cdot \frac{\tan \varphi}{|\tan \psi|} \cdot \frac{1 + \tan^{2}\psi}{1 + \tan^{2}\varphi} \cos(\varphi - |\psi|) - 1 \right]. \tag{38}$$

In case (a), from (29), we obtain

$$\frac{1 + \tan^2 \psi}{1 + \tan^2 \varphi} \le \frac{1 + (\tan \varphi + a)^2}{1 + \tan^2 \varphi} = 1 + a \cdot \frac{2 \tan \varphi + a}{1 + \tan^2 \varphi} \le 1 + a(1 + a). \tag{39}$$

Now, (38), (28) and (39) yield

$$\omega_{i\varphi} \le \frac{1}{g_{ii}} \left[\frac{g_{ii}}{g_{jj}} \cdot \frac{g_{jj}}{g_{ii}} \cdot (1 + a(1+a)) - 1 \right] = \frac{1}{g_{ii}} \cdot a(1+a) < \frac{1}{g_{ii}} \cdot \frac{a}{1-a}.$$

In case (b1), from (38), (32) and (30), we obtain

$$\omega_{i\varphi} \le \frac{1}{g_{ii}} \left[\frac{g_{ii}}{g_{jj}} \cdot \frac{g_{jj}}{g_{ii}} \cdot \frac{1}{1-a} - 1 \right] \le \frac{1}{g_{ii}} \cdot \frac{a}{1-a}.$$

In case (b2), from (38), (33) and (37), we obtain

$$\omega_{i\varphi} \le \frac{1}{g_{ii}} \left[\frac{g_{ii}}{g_{jj}} \cdot \frac{g_{jj}}{g_{ii}} \cdot \left(1 + a(1+a) \right) - 1 \right] \le \frac{1}{g_{ii}} \cdot a(1+a) < \frac{1}{g_{ii}} \cdot \frac{a}{1-a}.$$

Bound for $\omega_{i\varphi}$. From (18), we obtain

$$\begin{split} \omega_{j\varphi} &= \frac{c_{\varphi}^2}{g_{jj}c_{\psi}/c_{\varphi}} + \frac{s_{\varphi}^2}{g_{jj}|s_{\psi}|/s_{\varphi}} - \frac{1}{g_{jj}} = \frac{1}{g_{jj}} \left[\frac{c_{\varphi}^3}{c_{\psi}} + \frac{s_{\varphi}^3}{|s_{\psi}|} - 1 \right] \\ &= \frac{1}{g_{jj}} \left[\frac{c_{\varphi}}{c_{\psi}} \cdot c_{\varphi}^2 \cdot \left(1 + \frac{s_{\varphi}^2}{c_{\varphi}^2} \cdot \frac{s_{\varphi}/c_{\varphi}}{|s_{\psi}|/c_{\psi}} \right) - 1 \right] \\ &= \frac{1}{g_{jj}} \left[\sqrt{\frac{1 + \tan^2 \psi}{1 + \tan^2 \varphi}} \cdot \frac{1}{1 + \tan^2 \varphi} \cdot \left(1 + \tan^2 \varphi \frac{\tan \varphi}{|\tan \psi|} \right) - 1 \right]. \end{split}$$

In case (a), from (26) and (39), it follows that

$$\omega_{j\varphi} \le \frac{1}{g_{jj}} \left[\sqrt{1 + a(1+a)} \cdot \frac{1}{1 + \tan^2 \varphi} \cdot (1 + \tan^2 \varphi) - 1 \right]$$

$$\le \frac{1}{g_{jj}} \left[1 + a(1+a) - 1 \right] < \frac{1}{g_{jj}} \cdot \frac{a}{1 - a}.$$

In case (b1), from (30) and (32), we have

$$\omega_{j\varphi} \le \frac{1}{g_{jj}} \left[\frac{1}{1 + \tan^2 \varphi} \cdot \left(1 + \tan^2 \varphi \cdot \frac{1}{1 - a} \right) - 1 \right]$$
$$= \frac{1}{g_{jj}} \cdot \frac{\tan^2 \varphi}{1 + \tan^2 \varphi} \cdot \frac{a}{1 - a} < \frac{1}{g_{jj}} \cdot \frac{a}{1 - a}.$$

In case (b2), from (33), we obtain

$$\omega_{j\varphi} \leq \frac{1}{g_{jj}} \left[\frac{1}{1 + \tan^2 \varphi} \cdot \left(1 + \tan^2 \varphi \cdot \frac{\tan \varphi}{\tan \psi} \right) - 1 \right]$$

$$= \frac{1}{g_{jj}} \left[\frac{1}{1 + \tan^2 \varphi} \cdot \left(1 + \tan^2 \varphi - \tan^2 \varphi + \tan^2 \varphi \cdot \frac{\tan \varphi}{\tan \psi} \right) - 1 \right]$$

$$= \frac{1}{g_{jj}} \left[1 + \left(\frac{\tan \varphi}{\tan \psi} - 1 \right) \cdot \frac{\tan^2 \varphi}{1 + \tan^2 \varphi} - 1 \right]$$

$$= \frac{1}{g_{jj}} \left(\tan \varphi - \tan \psi \right) \cdot \frac{\tan \varphi}{\tan \psi} \cdot \frac{\tan \varphi}{1 + \tan^2 \varphi}.$$

Now, (34), (36), (35) and (33) yield

$$\omega_{j\varphi} \le \frac{1}{g_{jj}} \cdot a \cdot \sqrt{\frac{g_{ii}}{g_{jj}}} \cdot \frac{g_{jj}}{g_{ii}} \left(1 + a \tan \varphi\right) \cdot \sqrt{\frac{g_{ii}}{g_{jj}}} \cdot \frac{a + \tan \psi}{1 + \tan^2 \varphi}$$

$$= \frac{1}{g_{jj}} \cdot \frac{a(1 + a \tan \varphi)(a + \tan \varphi)}{1 + \tan^2 \varphi} = \frac{1}{g_{jj}} \cdot a \cdot \left[a + (1 + a^2) \frac{\tan \varphi}{1 + \tan^2 \varphi}\right]$$

$$\le \frac{1}{g_{jj}} \cdot a \cdot \frac{\left[a + (1 + a^2)\right](1 - a)}{1 - a} = \frac{1}{g_{jj}} \cdot a \cdot \frac{1 - a^3}{1 - a} < \frac{1}{g_{jj}} \cdot \frac{a}{1 - a}.$$

Bound for $|\omega_{\varphi}|$. From (18), we obtain

$$\omega_{\varphi} = 2s_{\varphi}c_{\varphi}\left(\frac{c_{\varphi}}{c_{\psi}g_{jj}} - \frac{s_{\varphi}}{|s_{\psi}|g_{jj}}\right) = \frac{1}{g_{jj}} \cdot 2s_{\varphi}c_{\varphi} \cdot \frac{c_{\varphi}}{c_{\psi}}\left(1 - \frac{s_{\varphi}/c_{\varphi}}{|s_{\psi}|/c_{\psi}}\right)$$
$$= \frac{1}{g_{jj}} \cdot \frac{2\tan\varphi}{1 + \tan^{2}\varphi} \cdot \frac{\cos\varphi}{\cos\psi} \cdot \left(1 - \frac{\tan\varphi}{|\tan\psi|}\right).$$

In case (a), from (26) and (29), we have

$$|\omega_{\varphi}| = \frac{1}{g_{jj}} \cdot \frac{2}{1 + \tan^2 \varphi} \cdot \frac{\sin \varphi}{|\sin \psi|} \cdot (|\tan \psi| - \tan \varphi) \le \frac{1}{g_{jj}} \cdot 2 \cdot \frac{|g_{ij}|}{g_{ii}}$$
$$= \frac{2}{g_{jj}} \cdot a \cdot \sqrt{\frac{g_{jj}}{g_{ii}}} = \frac{1}{\sqrt{g_{ii}g_{jj}}} \cdot 2a < \frac{1}{\sqrt{g_{ii}g_{jj}}} \cdot \frac{2a}{1 - a}.$$

In case (b1), (30) and (31) yield

$$\begin{aligned} |\omega_{\varphi}| &< \frac{1}{g_{jj}} \cdot \left(\frac{1}{1 - |g_{ij}|/g_{ii}} - 1\right) = \frac{1}{g_{jj}} \cdot \frac{|g_{ij}|/g_{ii}}{1 - |g_{ij}|/g_{ii}} \\ &= \frac{1}{g_{jj}} \cdot \frac{a\sqrt{g_{jj}/g_{ii}}}{1 - a\sqrt{g_{jj}/g_{ii}}} \le \frac{1}{g_{jj}} \cdot \frac{a\sqrt{g_{jj}/g_{ii}}}{1 - a} \le \frac{1}{\sqrt{g_{ii}g_{jj}}} \cdot \frac{a}{1 - a}. \end{aligned}$$

In case (b2), from (33), (36) and (34), we obtain

$$|\omega_{\varphi}| = \frac{1}{g_{jj}} \cdot \frac{2}{1 + \tan^{2} \varphi} \cdot \frac{\cos \varphi}{\cos \psi} \cdot \frac{\tan \varphi}{\tan \psi} \left(\tan \varphi - \tan \psi \right)$$

$$\leq \frac{1}{g_{jj}} \cdot \frac{2}{1 + \tan^{2} \varphi} \cdot \frac{g_{jj}}{g_{ii}} \left(1 + a \tan \varphi \right) \cdot a \cdot \sqrt{\frac{g_{ii}}{g_{jj}}}$$

$$= \frac{1}{\sqrt{g_{ii}g_{jj}}} \cdot 2a \cdot \left(\frac{1}{1 + \tan^{2} \varphi} + a \cdot \frac{\tan \varphi}{1 + \tan^{2} \varphi} \right)$$

$$\leq \frac{1}{\sqrt{g_{ii}g_{jj}}} \cdot 2a \cdot (1 + a) < \frac{1}{\sqrt{g_{ii}g_{jj}}} \cdot \frac{2a}{1 - a}.$$

Bound for $\omega_{i\psi}$. From (18), we obtain

$$\omega_{i\psi} = \frac{c_{\psi}^2 s_{\varphi}}{|s_{\psi}| |s_{\psi}|} + \frac{s_{\psi}^2 c_{\varphi}}{c_{\psi} g_{jj}} - \frac{1}{g_{ii}} = \frac{1}{g_{ii}} \left[\frac{g_{ii}}{g_{jj}} c_{\varphi} c_{\psi} \left(\frac{c_{\psi} s_{\varphi}}{|s_{\psi}| |c_{\varphi}|} + \frac{s_{\psi}^2}{c_{\psi}^2} \right) - 1 \right]$$
$$= \frac{1}{g_{ii}} \left[\frac{g_{ii}}{g_{jj}} \cos \varphi \cos \psi \cdot \left(\frac{\tan \varphi}{|\tan \psi|} + \tan^2 \psi \right) - 1 \right].$$

In case (a), from (26), (28) and (29), we have

$$\omega_{i\psi} < \frac{1}{g_{ii}} \left\{ \frac{g_{ii}}{g_{jj}} \cos^2 \varphi \cdot \left[\frac{g_{jj}}{g_{ii}} + \left(\frac{g_{jj}}{g_{ii}} \tan \varphi + \frac{|g_{ij}|}{g_{ii}} \right)^2 \right] - 1 \right\}$$

$$= \frac{1}{g_{ii}} \left\{ \frac{g_{ii}}{g_{jj}} \cos^2 \varphi \cdot \frac{g_{jj}}{g_{ii}} \left[1 + \left(\sqrt{\frac{g_{jj}}{g_{ii}}} \tan \varphi + a \right)^2 \right] - 1 \right\}$$

$$< \frac{1}{g_{ii}} \left\{ \cos^2 \varphi \left[1 + (\tan \varphi + a)^2 \right] - 1 \right\} = \frac{1}{g_{ii}} \left\{ \frac{1 + (\tan \varphi + a)^2}{1 + \tan^2 \varphi} - 1 \right\}$$

$$= \frac{1}{g_{ii}} \left\{ 1 + a \cdot \frac{2 \tan \varphi + a}{1 + \tan^2 \varphi} - 1 \right\} < \frac{1}{g_{ii}} \cdot a(1 + a) < \frac{1}{g_{ii}} \cdot \frac{a}{1 - a}.$$

In case (b1), (30) and (32) yield

$$\omega_{i\psi} = \frac{1}{g_{ii}} \left[\frac{g_{ii}}{g_{jj}} \cdot \left(\cos^2 \psi \frac{\sin \varphi}{\sin \psi} + \sin^2 \psi \frac{\cos \varphi}{\cos \psi} \right) - 1 \right]$$

$$< \frac{1}{g_{ii}} \left[\frac{g_{ii}}{g_{jj}} \cdot \left(\cos^2 \psi \frac{\sin \varphi}{\sin \psi} + \sin \varphi \sin \psi \right) - 1 \right] = \frac{1}{g_{ii}} \left[\frac{g_{ii}}{g_{jj}} \cdot \frac{\sin \varphi}{\sin \psi} - 1 \right]$$

$$= \frac{1}{g_{ii}} \left[\frac{g_{ii}}{g_{jj}} \cdot \frac{\tan \varphi}{\tan \psi} \cdot \frac{\cos \varphi}{\cos \psi} - 1 \right] \le \frac{1}{g_{ii}} \left[\frac{g_{ii}}{g_{jj}} \cdot \frac{g_{jj}}{g_{ii}} \cdot \frac{1}{1 - a} - 1 \right] = \frac{1}{g_{ii}} \cdot \frac{a}{1 - a}$$

In case (b2), similarly as above, from (33) and (37), we obtain

$$\omega_{i\psi} < \frac{1}{g_{ii}} \left[\frac{g_{ii}}{g_{jj}} \cdot \frac{\tan \varphi}{\tan \psi} \cdot \frac{\cos \varphi}{\cos \psi} - 1 \right] \le \frac{1}{g_{ii}} \left[\frac{g_{ii}}{g_{jj}} \cdot \frac{g_{jj}}{g_{ii}} \cdot \left(1 + a(1+a) \right) - 1 \right]$$

$$= \frac{1}{g_{ii}} \cdot a(1+a) < \frac{1}{g_{ii}} \cdot \frac{a}{1-a}.$$

Bound for $\omega_{i\psi}$. From (18), we obtain

$$\omega_{j\psi} = \frac{c_{\psi}^{2}}{g_{jj}c_{\psi}/c_{\varphi}} + \frac{s_{\psi}^{2}}{g_{jj}|s_{\psi}|/s_{\varphi}} - \frac{1}{g_{jj}} = \frac{1}{g_{jj}} (\cos\varphi\cos\psi + \sin\varphi|\sin\psi| - 1).$$

In case (a), from (26) and (29), we have

$$\omega_{j\psi} \le \frac{1}{g_{jj}} \left(\cos^2 \varphi + \sin \varphi |\sin \psi| - 1\right) = \frac{1}{g_{jj}} \sin \varphi \left(|\sin \psi| - \sin \varphi\right)$$

$$\le \frac{1}{g_{jj}} \cdot \left(\frac{|\tan \psi|}{\sqrt{1 + \tan^2 \psi}} - \frac{\tan \varphi}{\sqrt{1 + \tan^2 \varphi}}\right) < \frac{1}{g_{jj}} \cdot \frac{|\tan \psi| - \tan \varphi}{\sqrt{1 + \tan^2 \varphi}}$$

$$< \frac{1}{g_{jj}} \left(|\tan \psi| - \tan \varphi\right) < \frac{a}{g_{jj}} < \frac{1}{g_{jj}} \cdot \frac{a}{1 - a}.$$

In case (b1), in the same way as above, from (30) and (32), we have

$$\omega_{j\psi} < \frac{1}{g_{jj}} \left(\cos^2 \psi + \sin \varphi \sin \psi - 1 \right) = \frac{\sin \psi}{g_{jj}} \left(\sin \varphi - \sin \psi \right) \le \frac{1}{g_{jj}} \left(\tan \varphi - \tan \psi \right)$$
$$\le \frac{1}{g_{jj}} \tan \psi \left(\frac{1}{1-a} - 1 \right) \le \frac{1}{g_{jj}} \left(\frac{1}{1-a} - 1 \right) = \frac{1}{g_{jj}} \cdot \frac{a}{1-a}.$$

Similarly, in case (b2), from (33) and (35), we have

$$\omega_{j\psi} \le \frac{1}{g_{jj}} \left(\tan \varphi - \tan \psi \right) \le \frac{1}{g_{jj}} \cdot a < \frac{1}{g_{jj}} \cdot \frac{a}{1 - a}.$$

Bound for $|\omega_{\psi}|$. From (18), we obtain

$$\omega_{\psi} = 2s_{\psi}c_{\psi}\left(\frac{c_{\varphi}}{c_{\psi}g_{jj}} - \frac{s_{\varphi}}{|s_{\psi}|g_{jj}}\right) = \frac{2}{g_{jj}}\cos\varphi\cos\psi\cdot(\tan\psi - \operatorname{sign}s_{\psi}\tan\varphi).$$

In case (a), from (26) and (29), we have

$$|\omega_{\psi}| = \frac{2}{g_{jj}} \cos \varphi \cos \psi \cdot (|\tan \psi| - |\tan \varphi|) < \frac{2}{g_{jj}} \cdot \frac{|g_{ij}|}{g_{ii}}$$
$$= \frac{2}{g_{jj}} \cdot a \cdot \sqrt{\frac{g_{jj}}{g_{ii}}} = \frac{2a}{\sqrt{g_{ii}g_{jj}}} < \frac{1}{\sqrt{g_{ii}g_{jj}}} \cdot \frac{2a}{1-a}.$$

In case (b1), from (30) and (31), we have

$$|\omega_{\psi}| = \frac{2}{g_{jj}} \cos \varphi \sin \psi \cdot \left(\frac{\tan \varphi}{\tan \psi} - 1\right) < \frac{2}{g_{jj}} \cos \varphi \sin \varphi \cdot \left(\frac{1}{1 - |g_{ij}|/g_{ii}} - 1\right)$$
$$= \frac{\sin 2\varphi}{g_{ij}} \cdot \frac{|g_{ij}|/g_{ii}}{1 - |g_{ij}|/g_{ii}} = \frac{\sin 2\varphi}{g_{jj}} \cdot \frac{a\sqrt{g_{jj}/g_{ii}}}{1 - a\sqrt{g_{ij}/g_{ij}}} \le \frac{1}{\sqrt{g_{ii}g_{jj}}} \cdot \frac{a}{1 - a}.$$

In case (b2), from (35), we have

$$|\omega_{\psi}| = \frac{2}{g_{jj}} \cos \varphi \cos \psi \cdot (\tan \varphi - \tan \psi) < \frac{2}{\sqrt{g_{ii}g_{jj}}} \cdot a < \frac{1}{\sqrt{g_{ii}g_{jj}}} \cdot \frac{2a}{1 - a}.$$

Now, the obtained estimates for $\omega_{i\varphi}$, $\omega_{j\varphi}$, $|\omega_{\varphi}|$, $\omega_{i\psi}$, $|\omega_{j\psi}$, $|\omega_{\psi}|$, yield

$$\max\{\omega_{i\varphi}, \omega_{i\psi}\} < \frac{1}{g_{ii}} \cdot \frac{a}{1-a},$$

$$\max\{\omega_{j\varphi}, \omega_{j\psi}\} < \frac{1}{g_{jj}} \cdot \frac{a}{1-a},$$

$$\max\{|\omega_{\varphi}|, |\omega_{\psi}|\} < \frac{1}{\sqrt{g_{ii}g_{jj}}} \cdot \frac{2a}{1-a}.$$

$$(40)$$

From (25) and (40), we conclude that

$$(|\tilde{a}_{li}|^2 + |\tilde{a}_{lj}|^2) - (|a_{li}|^2 + |a_{lj}|^2) \le \frac{a}{1-a} |a_{li}|^2 + \frac{a}{1-a} |a_{lj}|^2 + \frac{2a}{1-a} |a_{li}a_{lj}|$$

$$= \frac{a}{1-a} (|a_{li}| + |a_{lj}|)^2$$

$$\le \frac{2a}{1-a} (|a_{li}|^2 + |a_{lj}|^2), \quad l \ne i, j,$$

which implies the assertion of Lemma 1, and thus completes the proof.

Note that the relation (40) holds for even and odd cycles, because the inequalities are symmetric in the arguments φ and ψ , and, therefore, invariant to their interchange. The next lemma bounds the growth of the off-norm of scaled matrices after one step.

Lemma 2. Let G_S and \widetilde{G}_S be as in Lemma 1. If $\|\Omega(\widetilde{G}_S)\| > \|\Omega(G_S)\|$, then

(i)
$$\|\Omega(\widetilde{G}_S)\|^2 - \|\Omega(G_S)\|^2 \le |a_{ij}| \cdot \frac{2\|\Omega(G_S)\|^2 - |a_{ij}|}{1 - |a_{ij}|},$$

$$|a_{ij}| \le 2||\Omega(G_S)||^2.$$

Proof. Since only the i-th and j-th row and column change, we can use Lemma 1 (see also the proof of [20, Lemma 2]) to obtain

$$\|\widetilde{A}\|^{2} - \|A\|^{2} = 2 \sum_{\substack{l=1\\l\neq i,j}}^{n} \left[(|\widetilde{a}_{il}|^{2} + |\widetilde{a}_{jl}|^{2}) - (|a_{il}|^{2} + |a_{jl}|^{2}) \right] - 2a_{ij}^{2}$$

$$\leq \frac{4|a_{ij}|}{1 - |a_{ij}|} \sum_{\substack{l=1\\l\neq i,j}}^{n} (|a_{il}|^{2} + |a_{jl}|^{2}) - 2a_{ij}^{2} \leq \frac{2|a_{ij}|}{1 - |a_{ij}|} (\|A\|^{2} - 2a_{ij}^{2}) - 2a_{ij}^{2}$$

$$= \frac{2|a_{ij}|}{1 - |a_{ij}|} (\|A\|^{2} - a_{ij}^{2} - |a_{ij}|) \leq \frac{2|a_{ij}|}{1 - |a_{ij}|} (\|A\|^{2} - |a_{ij}|),$$

which implies the assertions (i) and (ii), because

$$\|\widetilde{A}\|^2 = 2\|\Omega(\widetilde{G}_S)\|^2, \quad \|A\|^2 = 2\|\Omega(G_S)\|^2.$$

We are now able to bound the growth of α_k during one cycle of the method.

5. Asymptotic estimates

Here, we assume that $B^{(0)}$ is α_0 -scaled diagonally dominant, with α_0 sufficiently small for obtaining usable estimates of α_k , for all $1 \le k \le N$, where N = n(n-1)/2.

Lemma 3. Let $G^{(0)} = G$, $G^{(1)}, \ldots, G^{(N)}$ be obtained by applying N Kogbetliantz steps to G, and let α_k , $0 \le k \le N$, be defined by (22). If

$$\alpha_0 \le \frac{1}{10n}, \quad n \ge 3,\tag{41}$$

then

$$\alpha_k^2 \le c_k \alpha_0^2, \quad 0 \le k \le N, \tag{42}$$

where

$$c_k = \left(1 + \frac{0.011}{n^2}\right)^k < 1.006, \quad 0 \le k \le N.$$
 (43)

Proof. The proof is analogous to the proof of [20, Lemma 3] with a suitable modification of constants.

First, we prove (43). Since c_k increases with k, by using the known inequality $(1+x)^m < 1/(1-mx)$, which holds for all x, m > 0 such that mx < 1, we obtain

$$c_k \le c_N = \left(1 + \frac{0.011}{n^2}\right)^N \le \frac{1}{1 - \frac{0.011}{n^2} \cdot \frac{n(n-1)}{2}} < \frac{1}{1 - 0.0055} < 1.005531.$$
 (44)

The inequality (42) is proved by induction with respect to k. For k = 0 the inequality holds trivially. Suppose that it holds for some $0 \le k < N$. Then, from (41) and (44), we have

$$\alpha_k^2 \le c_k \alpha_0^2 \le \frac{1.005531}{100n^2} \le 0.01005531 \frac{1}{n^2} < 0.001118.$$
 (45)

It suffices to prove the induction step only for $\alpha_{k+1} > \alpha_k$. By Lemma 2 (i), we have

$$\alpha_{k+1}^2 - \alpha_k^2 \le |a_{ij}^{(k)}| \cdot \frac{2\alpha_k^2 - |a_{ij}^{(k)}|}{1 - |a_{ij}^{(k)}|}.$$
 (46)

The function

$$f(a) = a \frac{2\alpha_k^2 - a}{1 - a}, \quad a \in [0, 2\alpha_k^2],$$

attains its maximum at

$$a_* = \frac{2\alpha_k^2}{1 + \sqrt{1 - 2\alpha_k^2}}, \text{ and } f(a_*) = \frac{4\alpha_k^4}{\left(1 + \sqrt{1 - 2\alpha_k^2}\right)^2}.$$

From (46) and (45), we have

$$\alpha_{k+1}^2 \le \alpha_k^2 + f(a_*) < \alpha_k^2 \left(1 + \frac{4\alpha_k^2}{\left(1 + \sqrt{1 - 2 \cdot 0.001118}\right)^2} \right).$$

From this relation and the third inequality in (45), we obtain

$$\alpha_{k+1}^2 \le c_k \alpha_0^2 \left(1 + 1.00112 \cdot \frac{0.01005531}{n^2} \right) \le c_{k+1} \alpha_0^2,$$

which completes the induction step and the proof of the lemma.

Let $N_t = t(t-1)/2$, $2 \le t \le n$. The next result is closely related with the content of the last section. It estimates the growth of the affected part of column t, after N_{t-1} Kogbetliantz rotations under the column-cyclic pivot strategy. Note that after N_{t-1} steps, each element at position (r, s), $1 \le r < s < t$, has once been the pivot element.

Lemma 4. Let $G^{(0)} = G$, $G^{(1)}, \ldots, G^{(N)}$ be obtained by applying N Kogbetliantz steps to G under the column-cyclic strategy. Let

$$a_t^{(k)} = \left[a_{1t}^{(k)}, \dots, a_{t-1,t}^{(k)} \right]^T, \quad 2 \le t \le n, \quad 0 \le k \le N.$$

If $\alpha_0 \leq 1/(10n)$, then

$$\|a_t^{(N_{t-1})}\|^2 \le C_t \|a_t^{(0)}\|^2$$

where
$$C_t = [(1+\alpha)/(1-\alpha)]^{-(2t-5)} < 1.565$$
, with $\alpha = \sqrt{1.006} \alpha_0$.

Proof. The proof is similar to the proof of [20, Lemma 9]. Since we use Lemma 1 here, instead of the term $\mu = 1/(1-b)$, we have $\mu = (1+b)/(1-b)$, where

$$b = \max \left\{ \frac{|g_{i(k)j(k)}^{(k)}|}{\sqrt{g_{i(k)i(k)}^{(k)}g_{j(k)j(k)}^{(k)}}}, \quad 0 \le k < N_{t-1} \right\}.$$

In exactly the same way as in the proof of [20, Lemma 9], we obtain

$$||a_t^{(N_{t-1})}||^2 \le \mu^{2t-5} ||a_t^{(0)}||^2 = \left(\frac{1+b}{1-b}\right)^{2t-5} ||a_t^{(0)}||^2.$$

Using the inequality $(1+x)^m < 1/(1-mx)$ again, we have

$$\left(\frac{1+b}{1-b}\right)^{2t-5} \le \left(1 + \frac{2b}{1-b}\right)^{2(n-1)} \le \left(1 - \frac{2(n-1)b}{1-b}\right)^{-2}$$
$$= \left(1 + \frac{2(n-1)b}{1+b-2nb}\right)^2 \le \left(1 + \frac{2nb}{1-2nb}\right)^2 < 1.565.$$

In the last inequality we have used Lemma 3 and the asymptotic assumption to estimate $nb \le n\alpha \le n\alpha_0 \sqrt{1.006} \le \sqrt{1.006}/10$.

6. An application

Here we briefly sketch the quadratic convergence proof for scaled iterates by the serial Kogbetliantz method for triangular matrices in the case of simple singular values. The proof is too long to be presented here. It uses the technique from [20], and all the results from previous sections are used. A complete proof, together with numerical tests and discussion, will be published elsewhere.

Asymptotic assumptions

Let the initial triangular matrix $B \in \mathbb{C}^{n \times n}$ satisfy the following asymptotic assumptions (cf. the assumptions (A1) and (A2) from [20]):

(B1)
$$\alpha_0 \le \frac{1}{10} \min\left\{\frac{1}{n}, \theta\right\}, \quad n \ge 3,$$

(B2)
$$b_{11} > b_{22} > \dots > b_{nn} > 0,$$

where α_0 and θ are defined by (22) and (6), respectively. Note that (B1) includes the condition (8), so that Theorem 1 can be used. From (22), we see that the elements b_{rr} in (B2) can be replaced by g_{rr} , for $1 \le r \le n$. The assumptions (B1) and (B2) are sufficient conditions for proving the quadratic convergence of scaled iterates per cycle.

Auxiliary results

First, we find fixed intervals that contain the diagonal elements during the whole process, and then we estimate the rotation angles. We recall that i = i(k) and j = j(k) stand for pivot indices, and k numbers the steps.

Lemma 5. Let the sequence $G^{(k)} = (g_{lm}^{(k)})$, $k \geq 0$, be obtained by the associated Kogbetliantz process. If $G^{(0)}$ satisfies the asymptotic assumptions (B1) and (B2), then the following relations hold for $0 \leq k \leq N$:

$$(i) \qquad \left(1 - \frac{\theta}{49}\right)\sigma_t < g_{tt}^{(k)} < \left(1 + \frac{\theta}{49}\right)\sigma_t, \quad 1 \le t \le n,$$

(ii)
$$\operatorname{rg}(g_{tt}^{(k)}, g_{qq}^{(k)}) > \frac{24}{25}\theta, \quad t \neq q,$$

(iii)
$$\max\{|\tan\psi^{(k)}|, |\tan\varphi^{(k)}|\} \le \frac{|g_{ij}^{(k)}|}{g_{ii}^{(k)} - g_{jj}^{(k)}} \le \frac{25|a_{ij}^{(k)}|}{48\theta},$$

where $rg(\cdot,\cdot)$ and $a_{ij}^{(k)}$ are defined by the relations (3) and (21), respectively.

Next, we estimate the elements of column t, when the annihilations in this column take place.

Lemma 6. Let B satisfy the assumptions (B1) and (B2). Let the sequence $B^{(k)}$, $k \geq 0$, be generated by the column-cyclic Kogbetliantz method. Let $t \in \{2, ..., n\}$ and $\nu = N_{t-1}$. Then

(i)
$$a_{kt}^{(\nu+k)} = 0, \quad k = 1, \dots, t-1$$

$$(ii) \quad \left| a_{lt}^{(\nu+k)} \right| \le \sqrt{1.006} \left(\left| a_{lt}^{(\nu)} \right| + \frac{25}{24\theta} \sum_{r=1}^{k} \left| a_{lr}^{(\nu)} a_{rt}^{(\nu+r-1)} \right| \right),$$

$$k = 1, \dots, l - 1, \quad 2 \le l \le t - 1,$$

$$(iii) \quad \left| a_{lt}^{(\nu+k)} \right| \leq \frac{1.045}{\theta} \sum_{r=l+1}^{k} \left| a_{rt}^{(\nu+r-1)} \right| \cdot \left(\left| a_{lr}^{(\nu)} \right| + \frac{0.27}{\theta} \left| a_{lt}^{(\nu+l-1)} a_{rt}^{(\nu+l-1)} \right| \right),$$

$$k = l + 1, \dots, t - 2, \quad 1 \le l \le t - 2,$$

$$|a_{lm}^{(\nu+k)}| \le |a_{lm}^{(\nu)}| + \frac{25}{48\theta} \Big(|a_{lt}^{(\nu+l-1)} a_{mt}^{(\nu+l-1)}| + |a_{lt}^{(\nu+m-1)} a_{mt}^{(\nu+m-1)}| \Big),$$

$$k = \max\{l, m\}, \dots, t-1, \quad 1 \le l \ne m \le t-2.$$

By using Lemma 6, we can estimate the elements of the t-th column prior to, and after their annihilations. We use the following notation:

 $A_t^{(k)} = E_t^T A^{(k)} E_t$, where $E_t = [e_1, \dots, e_t], \ 2 \le t \le n$, i.e., $A_t^{(k)}$ is the leading principal submatrix of $A^{(k)}$ of order t;

 $a_t^{(k)} = \left[a_{1t}^{(k)}, \dots, a_{t-1,t}^{(k)}\right]^T \text{ is the upper triangular part of the column } t \text{ of } A^{(k)}, \text{ i.e.,}$ the upper triangular part of the last column of $A_t^{(k)}$.

Lemma 7. If the conditions of Lemma 6 are met, then for each $1 \le l \le t-1$ holds

(i)
$$\sum_{l=1}^{t-1} \left(a_{lt}^{(\nu+p_l)} \right)^2 \le \rho_t^2 \| a_t^{(\nu)} \|^2, \quad 0 \le p_l \le l-1,$$

$$(ii) \sum_{l=1}^{t-1} \left(a_{lt}^{(\nu+p_l)} \right)^2 \le \frac{0.55}{\theta^2} \rho_t^2 \|a_t^{(\nu)}\|^2 \left(\|A_{t-1}^{(\nu)}\|_F + \frac{0.39}{\theta} \rho_t^2 \|a_t^{(\nu)}\|^2 \right)^2, \quad l \le p_l \le t-1,$$

where

$$\rho_t = \frac{\sqrt{1.006}}{1 - 0.74/\theta \cdot \|A_{t-1}^{(\nu)}\|_F}.$$

Lemma 5, Lemma 6, and Lemma 7 are used to derive the quadratic convergence bound for scaled iterates.

The main theorem

We state here the main quadratic convergence result.

Theorem 2. Let $B \in \mathbb{C}^{n \times n}$ be a triangular matrix satisfying the asymptotic assumptions (B1) and (B2). Let the sequence $B^{(0)} = B, B^{(1)}, \ldots, B^{(N)}$ be generated by the column-cyclic Kogbetliantz method. Then

$$\frac{\alpha_N}{\theta} \le \left(\frac{11}{10} \cdot \frac{\alpha_0}{\theta}\right)^2,$$

where α_0 , α_N , and θ are defined by (22), and (6), respectively.

This result confirms the resemblance between the Hermitian Jacobi method and the Kogbetliantz method for triangular matrices (see also [3, 12, 13]). It can be used in predicting the number of sweeps till convergence. The main advantage of this result over the classical results lies in the fact that the relative gap θ need not be tiny, when the singular values cluster around zero. It is well-known that the classical results are often useless in such a case.

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