Note on the Quadratic Convergence of Kogbetliantz's Algorithm for Computing the Singular Value Decomposition

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ABSTRACT

This note is concerned with the quadratic convergence of Kogbetliantz algorithm for computing the singular value decomposition of a triangular matrix in the case of repeated or clustered singular values.

1. INTRODUCTION

The idea of using different rotations on each side of a matrix A in order to compute the singular value decomposition of A was first suggested by Kogbetliantz [3] and analysed by Forsythe and Henrici [2]. Forsthye and Henrici have proved the convergence of the cyclic Kogbetliantz algorithm under the assumption that all pairs of rotation angles $\{\phi_k, \psi_k\}$ lie in a closed interval $J \subset (-\pi/2, \pi/2)$ independent of k:

$$\phi_k, \psi_k \in J, \qquad k = 1, 2 \dots . \tag{1}$$

In a recent paper, Paige and Van Dooren [4] have shown that the cyclic Kogbetliantz algorithm ultimately converges quadratically when no pathologically close singular values are present.

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Since efficiency can often be gained in computing the SVD if the input matrix is first orthogonally transformed into triangular form [1], it has been suggested that the matrix be preprocessed by computing its QR decomposition, before using Kogbetliantz algorithm to compute its SVD. This note is concerned with the asymptotic quadratic convergence of cyclic Kogbetliantz algorithm for computing the SVD of a triangular matrix in the case of repeated or clustered singular values. We have assumed that the cyclic Kogbetliantz algorithm is convergent.

In this note, $\|\cdot\|_F$ and $\|\cdot\|_2$ denote Frobenius and 2-norm respectively, and $s(A)$ denotes the sum of squares of the off-diagonal elements of matrix A. $s_l(A)$ $[s_u(A)]$ is the sum of squares of the strictly lower [upper] triangular elements of A.

2. DESCRIPTION OF THE ALGORITHM OF KOGBETLIANTZ

Let A be a $n \times n$ real matrix, and let

$$A = U\Sigma V^T \tag{2}$$

be the SVD of A. The algorithm of Kogbetliantz for computing the decomposition (2) is based on the following observation. Let a_{ij} and a_{ji} be two off-diagonal elements of A. Let the rotation matrices

$$\hat{U}_k = \begin{pmatrix} \cos\phi_k & \sin\phi_k \\ -\sin\phi_k & \cos\phi_k \end{pmatrix} \tag{3}$$

and

$$\hat{V}_k = \begin{pmatrix} \cos\psi_k & \sin\psi_k \\ -\sin\psi_k & \cos\psi_k \end{pmatrix} \tag{4}$$

be chosen such that

$$\hat{U}_k \begin{pmatrix} a_{ii} & a_{ij} \\ a_{ji} & a_{jj} \end{pmatrix} \hat{V}_k = \begin{pmatrix} \hat{a}_{ii} & 0 \\ 0 & \hat{a}_{jj} \end{pmatrix} \tag{5}$$

is the SVD of the 2×2 submatrix subtended by the rows and columns i and j of A. The rotations of (3) and (4) can be constructed to satisfy (1) and (5) simultaneously [2]. Let U_k and V_k be the unit matrix with the elements $(i,i),(i,j),(j,i),(j,j)$ replaced by the elements $(1,1),(1,2),(2,1),(2,2)$ of $\hat{U}_k$ and $\hat{V}_k$, respectively; then $A_{k+1}=U_k^T A_k V_k$ satisfies

$$s(A_{k+1}) = s(A_k) - a_{ij}^2 - a_{ji}^2. \tag{6}$$

In this scheme, a sweep consists of zeroing the off-diagonal elements in the natural row ordering. For example with $n=4$, this is

$$(i,j) = (1,2),(1,3),(1,4),(2,3),(2,4),(3,4).$$

We will call the Kogbetliantz algorithm with row ordering *the cyclic Kogbetliantz algorithm.*

Heath et al. [5] discuss in detail the effect of the cyclic Kogbetliantz algorithm on a triangular matrix. They show that an upper triangular matrix A, after the first sweep, becomes lower triangular. The second sweep puts it back to upper triangular form, and so on. Moreover, it is easy to show that if A is an upper trapezoidal matrix of the form

$$A = \begin{pmatrix} A_{11} & A_{12} \\ 0 & 0 \end{pmatrix},$$

where A_{11} is nonsingular, then after the second sweep, it has the form

$$A_2 = \begin{pmatrix} A_{11}^{(2)} & 0 \\ 0 & 0 \end{pmatrix},$$

where $A_{11}^{(2)}$ is nonsingular upper triangular. So without loss of generality, we may assume that A is a nonsingular triangular matrix.

3. MAIN RESULT AND PROOF

This section gives a proof of the asymptotic quadratic convergence of the cyclic Kogbetliantz algorithm in the case of repeated or clustered singular values. We begin our formal development with a lemma.

LEMMA 3.1. *Let the* 2×2 *nonsingular upper triangular matrix*

$$\begin{pmatrix} a_{11} & a_{12} \\ 0 & a_{22} \end{pmatrix}$$

satisfy $|a_{11}| = \epsilon$, $|a_{11}|, |a_{22}| \gg \epsilon$, ϵ *is small. Let*

$$R_{12}P_{12}\begin{pmatrix} a_{11} & a_{12} \\ 0 & a_{22} \end{pmatrix}P_{12} = \begin{pmatrix} \hat{a}_{22} & \hat{a}_{12} \\ 0 & \hat{a}_{11} \end{pmatrix}, \tag{7}$$

where P_{12} *is a permutation and* R_{12} *a rotation. Then for any* σ_1, σ_2 *we have*

$$|\sigma_1 - \hat{a}_{11}| \leqslant |\sigma_1 - a_{11}| + O(\epsilon^2)\frac{|a_{11}|}{|a_{22}|^2} \tag{8}$$

and

$$|\sigma_2 - \hat{a}_{22}| \leqslant |\sigma_2 - a_{22}| + O(\epsilon^2)\frac{1}{|a_{22}|}. \tag{9}$$

Proof. Let the rotation have the form

$$R_{12} = \begin{pmatrix} c & s \\ -s & c \end{pmatrix}.$$

Then from (7), we know that $c = a_{22}/h$, $s = a_{12}/h$, where $h = \operatorname{sign}(a_{22})\sqrt{a_{22}^2 + a_{12}^2}$. Since $|a_{12}| = \epsilon$, and ϵ is small, it follows that

$$h = \sqrt{a_{22}^2 + \epsilon^2} = |a_{22}| + \frac{O(\epsilon^2)}{|a_{22}|}$$

and

$$\frac{1}{h} = \frac{1}{|a_{22}|} + \frac{O(\epsilon^2)}{|a_{22}^2|}.$$

From (7), we know that for any σ_1, σ_2

$$\begin{aligned}|\sigma_1 - \hat{a}_{11}| &= |\sigma_1 - a_{11}c| \\ &\leqslant |\sigma_1 - a_{11}| + |a_{11}|\,|1-c| \\ &\leqslant |\sigma_1 - a_{11}| + O(\epsilon^2)\frac{|a_{11}|}{|a_{22}|^2}\end{aligned}$$

and

$$\begin{aligned}|\sigma_2 - \hat{a}_{22}| &= |\sigma_2 - h| \\ &\leqslant |\sigma_2 - a_{22}| + O(\epsilon^2)\frac{1}{|a_{22}|},\end{aligned}$$

which is the desired result. ■

The lemma essentially tells us that if $a_{11} \to \sigma_1$, $a_{22} \to \sigma_2$, and σ_1 and σ_2 are reasonably separated, then on symmetric permutation and premultiplying with a rotation matrix, the new $\hat{a}_{11}$ and $\hat{a}_{22}$ will still converge to σ_1 and σ_2 respectively.

For proving the quadratic convergence in the case of repeated or clustered singular values, we suppose that all the a_{ii} which converge to repeated or clustered singular values σ are at the bottom of A's diagonal. This can always be obtained by a suitable reordering, but it not automatically obtained by the cyclic Kogbetliantz algorithm. We can then partition A accordingly as

$$A = \begin{pmatrix} A_{11} & A_{12} \\ 0 & A_{22} \end{pmatrix}, \tag{10}$$

where both A_{11} and A_{22} are upper triangular, and $A_{22} \to \sigma I$, and the off-diagonal elements of A satisfy

$$\|E\|_F < \eta, \tag{11}$$

where η is small. We illustrate how to obtain (10) for $n = 5$. Suppose $a_{11} \to \sigma_1$, $a_{55} \to \sigma_1$, and other diagonal elements converge to distinct singular values. By the preceding lemma, we can put a_{11} and a_{55} at the bottom of A's diagonal through symmetric permutation and premultiplying with appropriate rotation:

$$A \to P_{12}\begin{pmatrix} 1 & x & x & x & x \\ 0 & 2 & x & x & x \\ 0 & 0 & 3 & x & x \\ 0 & 0 & 0 & 4 & x \\ 0 & 0 & 0 & 0 & 5 \end{pmatrix} P_{12} \to R_{12}\begin{pmatrix} 2 & 0 & x & x & x \\ x & 1 & x & x & x \\ x & 1 & x & x & x \\ 0 & 0 & 3 & x & x \\ 0 & 0 & 0 & 4 & x \\ 0 & 0 & 0 & 0 & 5 \end{pmatrix}$$

$$\to P_{23}\begin{pmatrix} 2 & x & x & x & x \\ 0 & 1 & x & x & x \\ 0 & 0 & 3 & x & x \\ 0 & 0 & 0 & 4 & x \\ 0 & 0 & 0 & 0 & 5 \end{pmatrix} P_{23} \to P_{23}\begin{pmatrix} 2 & x & x & x & x \\ 0 & 3 & 0 & x & x \\ 0 & x & 1 & x & x \\ 0 & 0 & 0 & 4 & x \\ 0 & 0 & 0 & 0 & 5 \end{pmatrix}$$

$$\to P_{34}\begin{pmatrix} 2 & x & x & x & x \\ 0 & 3 & x & x & x \\ 0 & 0 & 1 & x & x \\ 0 & 0 & 0 & 4 & x \\ 0 & 0 & 0 & 0 & 5 \end{pmatrix} P_{34} \to R_{34}\begin{pmatrix} 2 & x & x & x & x \\ 0 & 3 & x & x & x \\ 0 & 0 & 4 & 0 & x \\ 0 & 0 & x & 1 & x \\ 0 & 0 & 0 & 0 & 5 \end{pmatrix},$$

where the indices indicate the position of the initial diagonal elements of matrix, and x represents the general matrix element. When treating the cyclic Kogbetliantz algorithm below, we will assume that a reordering step has been performed as soon as the cluster becomes apparent.

Starting from (10) with the cyclic Kogbetliantz algorithm, we have after one sweep

$$A_1 = D_1 + E_1 = \begin{pmatrix} \bar{A}_{11} & 0 \\ \bar{A}_{21} & \bar{A}_{22} \end{pmatrix}, \tag{12}$$

where D_1 is diagonal, E_1 is strictly lower triangular, $\bar{A}_{11}, \bar{A}_{22}$ are lower triangular, and $\bar{A}_{22} \to \sigma I$. Then

$$A_1^T A_1 = \begin{pmatrix} \bar{A}_{11}^T \bar{A}_{11} + \bar{A}_{21}^T \bar{A} & \bar{A}_{21}^T \bar{A}_{22} \\ \bar{A}_{22}^T \bar{A}_{21} & \bar{A}_{22}^T \bar{A}_{22} \end{pmatrix}, \tag{13}$$

and from the convergence of the cyclic Kogbetliantz algorithm,

$$\|F_1\|_F \leqslant \eta^2, \tag{14}$$

where F_1 is the strictly lower triangular part of $E_1^T E_1$. From (13), we have

$$A_1^T A_1 - \sigma^2 I = \begin{pmatrix} I & 0 \\ Z & I \end{pmatrix} \begin{pmatrix} X_\sigma & 0 \\ 0 & Y_\sigma \end{pmatrix} \begin{pmatrix} I & Z^T \\ 0 & I \end{pmatrix}, \tag{15}$$

where

$$X_\sigma = \bar{A}_{11}^T \bar{A}_{11} + \bar{A}_{21}^T \bar{A}_{21} - \sigma^2 I,$$

$$Y_\sigma = \bar{A}_{22}^T \bar{A}_{22} - \sigma^2 I - \bar{A}_{22}^T \bar{A}_{21} X_\sigma^{-1} \bar{A}_{21}^T \bar{A}_{22},$$

$$Z = \bar{A}_{21}^T \bar{A}_{21} X_\sigma^{-1}.$$

Now observe that the rank of $A_1^T A_1 - \sigma^2 I$ is $n - m$. By Sylvester's law of inertia (see e.g. [6]) the rank of the block diagonal factor must be $n - m$, and so $Y_\sigma = 0$. Thus

$$\bar{A}_{22}^T \bar{A}_{22} - \sigma^2 I = \bar{A}_{22}^T \bar{A}_{21} X_\sigma^{-1} \bar{A}_{21}^T \bar{A}_{22}. \tag{16}$$

By our assumption, we know that after a certain number of sweeps, all the singular values of $\bar{A}_{11}$ will be separated from σ by δ or more, in other words,

$$\rho \equiv \left\| \left(\bar{A}_{11}^T \bar{A}_{11} - \sigma^2 I \right)^{-1} \right\|_2 \leqslant \frac{1}{\min|\sigma_i - \sigma|} \leqslant \frac{1}{\delta}. \tag{17}$$

Thus from (16) and (17), we have

$$\begin{aligned} \sqrt{2}\, s_l^{1/2}\left(\bar{A}_{22}^T \bar{A}_{22} \right) &\leqslant \| \bar{A}_{22}^T \bar{A}_{22} - \sigma^2 I \|_F \\ &\leqslant \| \bar{A}_{22}^T \bar{A}_{21} \|_F^2 \| X_\sigma^{-1} \|_F \\ &\leqslant s_l\left(A_1^T A_1 \right) \rho \left\| \left[I + \bar{A}_{21}^T \bar{A}_{21} \left(\bar{A}_{11}^T \bar{A}_{11} - \sigma^2 I \right)^{-1} \right]^{-1} \right\|_F \\ &\leqslant s_l\left(A_1^T A_1 \right) \frac{1}{\delta} \frac{1}{1 - \| \bar{A}_{21} \|_F^2 / \delta} \\ &\leqslant s_l\left(A_1^T A_1 \right) \frac{1}{\delta} \frac{1}{1 - \eta^2/\delta}, \end{aligned}$$

i.e.,

$$\sqrt{2}\, s_l^{1/2}\left(\bar{A}_{22}^T \bar{A}_{22} \right) \leqslant \frac{1}{\delta - \eta^2} s_l\left(A_1^T A_1 \right) \tag{18}$$

This is the core inequality for proving the main result. In order to show the result more clearly, we need the following proposition.

PROPOSITION 3.2. *Denote a nonsingular lower triangular matrix A as*

$$A = D + E \tag{19}$$

where D is diagonal and E is triangular. Then there exist m and M such that

$$0 < m \leqslant d_{\min} \leqslant d_{\max} \leqslant M$$

and

$$\tfrac{1}{2}m^2 s_1(A) - \|F\|_F^2 \leqslant s_1(A^TA) \leqslant 2M^2 s_l(A) + 2\|F\|_F^2 \tag{20}$$

where $d_{\max}$ and $d_{\min}$ denote the largest and smallest elements of D respectively. F is a strictly lower triangular part of E^TE.

Proof. From (19), we know

$$\begin{aligned} A^TA &= (D+E)^T(D+E) \\ &= D^2 + DE + E^TD + E^TE. \end{aligned}$$

Let $E^TE = \Sigma + F + F^T$, where Σ is diagonal and F is a strictly lower triangular. Then

$$\begin{aligned} s_l(A^TA) &= \|DE + F\|_F^2 \\ &\leqslant (\|DE\|_F + \|F\|_F)^2 \\ &\leqslant 2(\|DE\|_F^2 + \|F\|_F^2) \\ &\leqslant 2M^2\|E\|_F^2 + 2\|F\|_F^2 \\ &= 2M^2 s_l(A) + 2\|F\|_F^2. \end{aligned}$$

On the other hand, since for arbitrary matrices A and B

$$\|A + B\|_F^2 \geqslant \tfrac{1}{2}\|A\|_F^2 - \|B\|_F^2,$$

we have

$$\begin{aligned} s_l(A^TA) &= \|DE+F\|_F^2 \\ &\geqslant \tfrac{1}{2}\|DE\|_F^2 - \|F\|_F^2 \\ &\geqslant \tfrac{1}{2}m^2\|E\|_F^2 - \|F\|_F^2 \\ &= \tfrac{1}{2}m^2 s_l(A) - \|F\|_F^2. \end{aligned}$$

Thus the proposition is proved. ■

Now, from (18) and (20) and the convergence of the Kogbetliantz algorithm, we know that there exist m_1, M_1, $0 < m_1 \leqslant \sigma_{\min} \leqslant \sigma_{\max} \leqslant M_1$, where $\sigma_{\min}$ and $\sigma_{\max}$ denote the smallest and largest singular values of A respectively, such that

$$s_l^{1/2}(\bar{A}_{22}) \leqslant \left(\frac{2}{\delta - \eta^2}\right)\frac{M_1^2}{m_1} s_l(A_1) + O(\eta^2). \tag{21}$$

And from (6), we know that

$$s_l(A_1) \leqslant s_u(A).$$

We then have

$$s_l^{1/2}(\bar{A}_{22}) \leqslant \left(\frac{2}{\delta - \eta^2}\right)\frac{M_1^2}{m_1} s_u(A) + O(\eta^2). \tag{22}$$

This shows that at some stage, after a sweep, the new off-diagonal elements will be the squares of the old ones. This behavior thus shows *asymptotic quadratic convergence.*

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