REORDERING DIAGONAL BLOCKS IN REAL SCHUR FORM

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Abstract

We present a direct algorithm for computing an orthogonal similarity transformation which interchanges neighboring diagonal blocks in a matrix in real Schur form. The algorithm does not require the solution of the associated Sylvester equation. Numerical tests suggest the backward stability of the scheme.

1 Introduction

The problem of reordering eigenvalues of a matrix in real Schur form arises in the computation of the invariant subspaces corresponding to a group of eigenvalues of the matrix. A basic step in such reordering is to swap two neighboring 1×1 or 2×2 diagonal blocks by an orthogonal transformation. Swapping two 1×1 blocks or swapping 1×1 and 2×2 blocks are well understood [3]. Swapping two 2×2 blocks poses some numerical difficulties. Recently, Bai and Demmel [1] have proposed an algorithm for swapping two 2×2 blocks which is for all practical purposes backward stable. The algorithm requires the solution of a Sylvester equation associated with the defining 4×4 matrix. If the algorithm introduces unacceptable rounding error in the (2,1) block of the transformed 4 matrix the interchange of the diagonal blocks is not performed. This can only happen if the eigenvalues of the two 2×2 blocks are almost identical and hence the interchange can be skipped. In this note we describe an alternative approach for swapping two 2×2 blocks which is based on an eigenvector calculation. It appears that the method guarantees small rounding errors in the (2,1) block of the transformed 4×4 matrix even if the two 2×2 blocks have almost the same eigenvalues.

2 Reordering eigenvalues

Assume that A is a 4×4 block triangular matrix,

$$A = \begin{pmatrix} A_{11} & A_{12} \\ 0 & A_{22} \end{pmatrix} = \begin{pmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ 0 & 0 & a_{33} & a_{34} \\ 0 & 0 & a_{43} & a_{44} \end{pmatrix}, \tag{2.1}$$

where A_{11} and A_{22} are 2×2 with pairs of complex conjugate eigenvalues λ_1, $\bar\lambda_1$ and λ_2, $\bar\lambda_2$. We can further assume that A_{11} and A_{22} are in the standard form,

$$A_{11} = \begin{pmatrix} \alpha_1 & \beta_1/k_1 \\ -\beta_1 k_1 & \alpha_1 \end{pmatrix} \quad and \quad A_{22} = \begin{pmatrix} \alpha_2 & \beta_2/k_2 \\ -\beta_2 k_2 & \alpha_2 \end{pmatrix} . \tag{2.2}$$

We want to find an orthogonal transformation Q such that

$$\hat A \equiv QAQ^T = \begin{pmatrix} \hat A_{11} & \hat A_{12} \\ 0 & \hat A_{22} \end{pmatrix} , \tag{2.3}$$

where $\hat A_{11}$ and $\hat A_{22}$ are similar to A_{22} and A_{11} respectively.

The standard form implies that $\lambda_2 = \alpha_2 + \beta_2 \cdot i$ is the eigenvalue of A_{22}. Thus $A(\lambda_2) = A - \lambda_2 \cdot I$ is singular as its (2,2) diagonal block has rank 1. Now one can find a sequence of complex Givens rotations such that

$$\begin{pmatrix} a_{11}-\lambda_2 & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22}-\lambda_2 & a_{23} & a_{24} \\ 0 & 0 & a_{33}-\lambda_2 & a_{34} \\ 0 & 0 & a_{43} & a_{44}-\lambda_2 \end{pmatrix} G_{34}^{(1)} G_{12}^{(2)} G_{23}^{(3)} G_{12}^{(4)} = \begin{pmatrix} 0^{(4)} & \tilde a_{12} & \tilde a_{13} & \tilde a_{14} \\ 0^{(2)} & 0^{(3)} & \tilde a_{23} & \tilde a_{24} \\ 0 & 0 & 0^{(1)} & \tilde a_{34} \\ 0 & 0 & 0^{(1)} & \tilde a_{44} \end{pmatrix} \tag{2.4}$$

where $G_{ij}^{(k)}$ denotes a complex Givens rotation operating in the plane (i , j) introducing zero at the position marked as (k) on the right hand side of the relation.

Let $G = G_{34}^{(1)} G_{12}^{(2)} G_{23}^{(3)} G_{12}^{(4)}$. Then $y = u + v \cdot i = Ge_1$, where $u = [u_1, u_2, u_3, u_4]^T$ and $v = [v_1, v_2, v_3, v_4]^T$ are real vectors, is the complex eigenvector corresponding to λ_2. Hence

$$\begin{pmatrix} A_{11} & A_{12} \\ 0 & A_{22} \end{pmatrix} (u \;\; v) = (u \;\; v) \begin{pmatrix} \alpha_2 & \beta_2 \\ -\beta_2 & \alpha_2 \end{pmatrix} . \tag{2.5}$$

Moreover, because A_{22} is assumed to be in a standard form, $u_4 = v_3 = 0$, and $k_2 = \frac{u_3}{v_4}$ in (2.2).

Consider a transformation Q in the form of a product of real Givens rotations which triangularizes the matrix $[u\; v]$. More precisely, let $J_{12}^{(1)}$, $J_{23}^{(2)}$, $J_{12}^{(3)}$, $J_{34}^{(4)}$ and $J_{23}^{(5)}$ be such that

$$(a) \quad J_{12}^{(1)} \begin{pmatrix} u_1 & v_1 \\ u_2 & v_2 \\ u_3 & 0 \\ 0 & v_4 \end{pmatrix} = \begin{pmatrix} u_1^{(1)} & v_1^{(1)} \\ u_2^{(1)} & 0^{(1)} \\ u_3 & 0 \\ 0 & v_4 \end{pmatrix} , \quad (b) \quad J_{23}^{(2)} \begin{pmatrix} u_1^{(1)} & v_1^{(1)} \\ u_2^{(1)} & 0^{(1)} \\ u_3 & 0 \\ 0 & v_4 \end{pmatrix} = \begin{pmatrix} u_1^{(1)} & v_1^{(1)} \\ u_2^{(2)} & 0^{(2)} \\ 0^{(2)} & 0^{(2)} \\ 0 & v_4 \end{pmatrix} ,$$

$$(c) \quad J_{12}^{(3)} \begin{pmatrix} u_1^{(1)} & v_1^{(1)} \\ u_2^{(2)} & 0^{(2)} \\ 0^{(2)} & 0^{(2)} \\ 0 & v_4 \end{pmatrix} = \begin{pmatrix} u_1^{(3)} & v_1^{(3)} \\ 0^{(3)} & v_2^{(3)} \\ 0^{(2)} & 0^{(2)} \\ 0 & v_4 \end{pmatrix} , \quad (d) \quad J_{34}^{(4)} \begin{pmatrix} u_1^{(3)} & v_1^{(3)} \\ 0^{(3)} & v_2^{(3)} \\ 0^{(2)} & 0^{(2)} \\ 0 & v_4 \end{pmatrix} = \begin{pmatrix} u_1^{(3)} & v_1^{(3)} \\ 0^{(3)} & v_2^{(3)} \\ 0^{(4)} & v_4^{(4)} \\ 0^{(4)} & 0^{(4)} \end{pmatrix} , \tag{2.6}$$

$$(e) \quad J_{23}^{(5)} \begin{pmatrix} u_1^{(3)} & v_1^{(3)} \\ 0^{(3)} & v_2^{(3)} \\ 0^{(4)} & v_4^{(4)} \\ 0^{(4)} & 0^{(4)} \end{pmatrix} = \begin{pmatrix} u_1^{(3)} & v_1^{(3)} \\ 0^{(5)} & v_2^{(5)} \\ 0^{(5)} & 0^{(5)} \\ 0^{(4)} & 0^{(4)} \end{pmatrix} ,$$

where $J_{ij}^{(k)}$ denotes a rotation operating in plane (i , j) and the superscript (k) corresponds to order in which the elements are affected by the rotation. Define the transformation Q as

$$Q = J_{23}^{(5)} J_{34}^{(4)} J_{12}^{(3)} J_{23}^{(2)} J_{12}^{(1)} .$$

It is easy to see that Q is the desired similarity transformation satisfying (2.3), that is

$$\hat{A} = Q \begin{pmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ 0 & 0 & a_{33} & a_{34} \\ 0 & 0 & a_{43} & a_{44} \end{pmatrix} Q^T = \begin{pmatrix} \hat{a}_{11} & \hat{a}_{12} & \hat{a}_{13} & \hat{a}_{14} \\ \hat{a}_{21} & \hat{a}_{22} & \hat{a}_{23} & \hat{a}_{24} \\ 0 & 0 & \hat{a}_{33} & \hat{a}_{34} \\ 0 & 0 & \hat{a}_{43} & \hat{a}_{44} \end{pmatrix} . \tag{2.7}$$

Moreover,

$$\begin{pmatrix} \hat{a}_{11} & \hat{a}_{12} & \hat{a}_{13} & \hat{a}_{14} \\ \hat{a}_{21} & \hat{a}_{22} & \hat{a}_{23} & \hat{a}_{24} \\ 0 & 0 & \hat{a}_{33} & \hat{a}_{34} \\ 0 & 0 & \hat{a}_{43} & \hat{a}_{44} \end{pmatrix} \begin{pmatrix} u_1^{(3)} & v_1^{(3)} \\ 0 & v_2^{(5)} \\ 0 & 0 \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} u_1^{(3)} & v_1^{(3)} \\ 0 & v_2^{(5)} \\ 0 & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} \alpha_2 & \beta_2 \\ -\beta_2 & \alpha_2 \end{pmatrix} . \tag{2.8}$$

3 Rounding error analysis

First we establish obvious relations tying the computed quantities which will play important roles in the analysis.

It is clear that the computed u and v satisfy a perturbed version of (2.5) namely

$$(A + \Delta A)\,(u \;\; v) = (u \;\; v) \begin{pmatrix} \alpha_2 & \beta_2 \\ -\beta_2 & \alpha_2 \end{pmatrix} , \quad ||\Delta A|| \le \epsilon \cdot ||A|| . \tag{3.1}$$

Denote by $\delta_{ij}^{(k)}$ the absolute error introduced in (i , j) position of the matrix $[u\, ,\, v]$ due to the application of the kth transformation $J_{pq}^{(k)}$. Then

$$Q \begin{pmatrix} u_1 & v_1 \\ u_2 & v_2 \\ u_3 & 0 \\ 0 & v_4 \end{pmatrix} = \begin{pmatrix} u_1^{(3)} & v_1^{(3)} \\ \delta_{21}^{(3)} & v_2^{(5)} \\ \delta_{31}^{(5)} & \delta_{32}^{(5)} \\ \delta_{41}^{(4)} & \delta_{42}^{(4)} \end{pmatrix} \tag{3.2}$$

where

$$|| \begin{pmatrix} \delta_{21}^{(3)} \\ \delta_{31}^{(5)} \\ \delta_{41}^{(2)} \end{pmatrix} || \le \epsilon \cdot |u_1^{(3)}| \quad , \quad || \begin{pmatrix} \delta_{32}^{(5)} \\ \delta_{42}^{(2)} \end{pmatrix} \le \epsilon \cdot || \begin{pmatrix} v_1^{(3)} \\ v_2^{(5)} \end{pmatrix} || . \tag{3.3}$$

Define $\bar{A}$ as follows

$$\bar{A} = Q(A + \Delta A)Q^T = \begin{pmatrix} \bar{a}_{11} & \bar{a}_{12} & \bar{a}_{13} & \bar{a}_{14} \\ \bar{a}_{21} & \bar{a}_{22} & \bar{a}_{23} & \bar{a}_{24} \\ \eta_{31} & \eta_{32} & \bar{a}_{33} & \bar{a}_{34} \\ \eta_{41} & \eta_{42} & \bar{a}_{43} & \bar{a}_{44} \end{pmatrix} . \tag{3.4}$$

We want to derive a bound on the norm of the (2,1) block $\bar{A}_{21}$,

$$\bar{A}_{21} = \begin{pmatrix} \eta_{31} & \eta_{32} \\ \eta_{41} & \eta_{42} \end{pmatrix} .$$

First note that $\bar{A}$ satisfies the relation

$$\begin{pmatrix} \bar{a}_{11} & \bar{a}_{12} & \bar{a}_{13} & \bar{a}_{14} \\ \bar{a}_{21} & \bar{a}_{22} & \bar{a}_{23} & \bar{a}_{24} \\ \eta_{31} & \eta_{32} & \bar{a}_{33} & \bar{a}_{34} \\ \eta_{41} & \eta_{42} & \bar{a}_{43} & \bar{a}_{44} \end{pmatrix} \begin{pmatrix} u_1^{(3)} & v_1^{(3)} \\ \delta_{21}^{(3)} & v_2^{(5)} \\ \delta_{31}^{(5)} & \delta_{32}^{(5)} \\ \delta_{41}^{(2)} & \delta_{42}^{(2)} \end{pmatrix} = \begin{pmatrix} u_1^{(3)} & v_1^{(3)} \\ \delta_{21}^{(3)} & v_2^{(5)} \\ \delta_{31}^{(5)} & \delta_{32}^{(5)} \\ \delta_{41}^{(2)} & \delta_{42}^{(2)} \end{pmatrix} \begin{pmatrix} \alpha_2 & \beta_2 \\ -\beta_2 & \alpha_2 \end{pmatrix} . \tag{3.5}$$

Recall that $||y|| = 1$ and hence $||u||$, $||v|| \leq 1$. For the purpose of analysis, assume without loss of generality that $|u_1^{(3)}| = ||u|| \geq ||v||$.

As $|\alpha_2|, |\beta_2| \leq ||A||$, the relation (3.5) together with (3.3) implies the inequality

$$||\begin{pmatrix} \eta_{31} \\ \eta_{41} \end{pmatrix}|| \leq \epsilon \cdot ||A|| , \tag{3.6}$$

which provides a bound on the norm of the first column of $\bar{A}_{21}$.

In order to obtain a bound on the norm of the second column of $\bar{A}_{21}$ note that the relation (3.5) implies

$$\begin{pmatrix} \eta_{31} \\ \eta_{41} \end{pmatrix} \cdot v_1^{(3)} + \begin{pmatrix} \eta_{32} \\ \eta_{42} \end{pmatrix} \cdot v_2^{(5)} + \begin{pmatrix} \bar{a}_{33} & \bar{a}_{34} \\ \bar{a}_{43} & \bar{a}_{44} \end{pmatrix} \begin{pmatrix} \delta_{32}^{(5)} \\ \delta_{42}^{(4)} \end{pmatrix} = \beta_2 \begin{pmatrix} \delta_{31}^{(5)} \\ \delta_{41}^{(4)} \end{pmatrix} + \alpha_2 \begin{pmatrix} \delta_{32}^{(5)} \\ \delta_{42}^{(4)} \end{pmatrix} \tag{3.7}$$

We have to consider two cases.

Case 1. The first case is when $|v_1^{(3)}| \leq |v_2^{(5)}|$. Then (3.7), (3.3) and (3.6) give

$$||\begin{pmatrix} \eta_{32} \\ \eta_{42} \end{pmatrix}|| \approx (\beta_2 \cdot \frac{|u_1^{(3)}|}{|v_2^{(5)}|}) \cdot \epsilon + \epsilon \cdot ||A|| . \tag{3.8}$$

By equating the elements in the position (1,2) on the both sides of (2.8) we obtain

$$\hat{a}_{11} v_1^{(3)} + \hat{a}_{12} v_2^{(5)} = u_1^{(3)} \beta_2 + v_1^{(3)} \alpha_2 , \tag{3.9}$$

from which it follows

$$|\beta_2 \cdot \frac{u_1^{(3)}}{v_2^{(5)}}| \leq |\hat{a}_{11}| + |\hat{a}_{12}| + |\alpha_2| \leq ||A|| . \tag{3.10}$$

¿From this and the relation (3.8) a bound on the norm of the second column of $\bar{A}_{21}$ of the form

$$||\begin{pmatrix} \eta_{32} \\ \eta_{42} \end{pmatrix}|| \leq \epsilon \cdot ||A|| , \tag{3.11}$$

can be derived and hence, because of (3.6), in Case 1 we always have

$$||\bar{A}_{21}|| \leq \epsilon \cdot ||A|| . \tag{3.12}$$

Case 2. The remaining case when $|v_1^{(3)}| > |v_2^{(5)}|$ requires more detailed considerations. Let $r = |\frac{v_2^{(5)}}{v_1^{(3)}}|$ Then $r < 1$. From the definition of the transformation $J_{23}^{(5)}$ we have

$$max(|v_2^{(3)}| , |v_4|) \leq |v_2^{(5)}| \leq r \cdot v_1^{(3)} . \tag{3.13}$$

Let the cosine-sine pair defining $J_{12}^{(3)}$ in (2.6)(c) be (c_3 , s_3). Then

$$\begin{pmatrix} c_3 & s_3 \\ -s_3 & c_3 \end{pmatrix} \begin{pmatrix} v_1^{(1)} \\ 0 \end{pmatrix} = \begin{pmatrix} v_1^{(3)} \\ v_2^{(3)} \end{pmatrix} \tag{3.14}$$

and hence

$$c_3 = \frac{v_1^{(3)}}{v_1^{(1)}} \quad and \quad s_3 = -\frac{v_2^{(3)}}{v_1^{(1)}} .$$

Now, from the relations (3.13) and (3.14) it follows that

$$|s_3| = |\frac{v_2^{(3)}}{v_1^{(1)}}| \leq |\frac{v_2^{(5)}}{v_1^{(3)}}| = r \; . \tag{3.15}$$

The cosine-sine pair defining $J_{12}^{(3)}$ in (2.6)(c) also satisfies the equality

$$\begin{pmatrix} c_3 & s_3 \\ -s_3 & c_3 \end{pmatrix} \begin{pmatrix} u_1^{(1)} \\ u_2^{(2)} \end{pmatrix} = \begin{pmatrix} u_1^{(3)} \\ 0 \end{pmatrix} \; .$$

and hence

$$c_3 = \frac{u_1^{(1)}}{u_1^{(3)}} \quad \textit{and} \quad s_3 = \frac{u_2^{(2)}}{u_1^{(3)}} \; .$$

Thus (3.15) implies

$$u_2^{(2)} \leq u_1^{(3)} \cdot s_3 \leq u_1^{(3)} \cdot r \; , \tag{3.16}$$

from which we obtain

$$|| \begin{pmatrix} \delta_{21}^{(3)} \\ \delta_{31}^{(5)} \\ \delta_{41}^{(2)} \end{pmatrix} || \leq r \cdot \epsilon \cdot |u_1^{(3)}| \quad , \tag{3.17}$$

Similarly, the relations (2.6)(d) and (2.6)(e) imply

$$|| \begin{pmatrix} \delta_{32}^{(5)} \\ \delta_{42}^{(2)} \end{pmatrix} || \leq \epsilon \cdot |v_2^{(5)}| \leq r \cdot \epsilon \cdot |v_1^{(3)}| \; . \tag{3.18}$$

¿From (3.5) we get

$$\begin{pmatrix} \eta_{31} \\ \eta_{41} \end{pmatrix} \cdot u_1^{(3)} + \begin{pmatrix} \eta_{32} \\ \eta_{42} \end{pmatrix} \cdot \delta_{21}^{(3)} + \begin{pmatrix} \bar{a}_{33} & \bar{a}_{34} \\ \bar{a}_{43} & \bar{a}_{44} \end{pmatrix} \begin{pmatrix} \delta_{31}^{(5)} \\ \delta_{41}^{(4)} \end{pmatrix} = \alpha_2 \begin{pmatrix} \delta_{31}^{(5)} \\ \delta_{41}^{(4)} \end{pmatrix} - \beta_2 \begin{pmatrix} \delta_{32}^{(5)} \\ \delta_{42}^{(4)} \end{pmatrix} \tag{3.19}$$

and thus due to (3.17) and (3.18)

$$|| \begin{pmatrix} \eta_{31} \\ \eta_{41} \end{pmatrix} || \leq r \cdot \epsilon \cdot ||A|| \; . \tag{3.20}$$

Similarly, for the second column of $\bar{A}_{21}$ from (3.5) we get

$$\begin{pmatrix} \eta_{31} \\ \eta_{41} \end{pmatrix} \cdot v_1^{(3)} + \begin{pmatrix} \eta_{32} \\ \eta_{42} \end{pmatrix} \cdot v_2^{(5)} + \begin{pmatrix} \bar{a}_{33} & \bar{a}_{34} \\ \bar{a}_{43} & \bar{a}_{44} \end{pmatrix} \begin{pmatrix} \delta_{32}^{(5)} \\ \delta_{42}^{(4)} \end{pmatrix} = \beta_2 \begin{pmatrix} \delta_{31}^{(5)} \\ \delta_{41}^{(4)} \end{pmatrix} + \alpha_2 \begin{pmatrix} \delta_{32}^{(5)} \\ \delta_{42}^{(4)} \end{pmatrix} \tag{3.21}$$

and thus due to (3.20)

$$|| \begin{pmatrix} \eta_{32} \\ \eta_{42} \end{pmatrix} || \approx (\beta_2 \cdot \frac{|u_1^{(3)}|}{|v_1^{(3)}|}) \cdot \epsilon + \epsilon \cdot ||A|| \; . \tag{3.22}$$

¿From the relation (3.9) we can derive a bound on $|\beta_2 \cdot \frac{|u_1^{(3)}|}{|v_1^{(3)}|}|$ of the form

$$|\beta_2 \cdot \frac{u_1^{(3)}}{v_1^{(3)}}| \leq |\hat{a}_{11}| + |\hat{a}_{12}| + |\alpha_2| \leq ||A|| \; . \tag{3.23}$$

This and the relations (3.6) and (3.22) imply that in Case 2 we always have

$$||\bar{A}_{21}|| \leq \epsilon \cdot ||A|| \; . \tag{3.24}$$

The relations (3.4), (3.12) and (3.24) imply that there exists a perturbation δA of A such that $||\delta A|| \leq \epsilon \cdot ||A||$ and

$$Q(A+\delta A)Q^T = \begin{pmatrix} \bar{a}_{11} & \bar{a}_{12} & \bar{a}_{13} & \bar{a}_{14} \\ \bar{a}_{21} & \bar{a}_{22} & \bar{a}_{23} & \bar{a}_{24} \\ 0 & 0 & \bar{a}_{33} & \bar{a}_{34} \\ 0 & 0 & \bar{a}_{43} & \bar{a}_{44} \end{pmatrix} . \tag{3.25}$$

$\square$

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