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A SIMPLE AUGMENTED JACOBI METHOD FOR HERMITIAN AND SKEW-HERMITIAN MATRICES

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Abstract. In this paper, we present a new extended Jacobi method for computing eigenvalues and eigenvectors of Hermitian matrices which does not use any complex arithmetics. This method can be readily applied to skew-Hermitian and real skew-symmetric matrices as well. An example illustrating its computational efficiency is given.

1. Introduction

In computing eigenvalues of matrices, there have been considerably much researches focused on the QR method [3] and the Jacobi method [6]. The QR method can be applied to general matrices, while the Jacobi method is restricted on real symmetric matrices. For the case of real symmetric matrices, it was shown that the Jacobi method performs better than the QR method [7]. Hacon in [4] extended the Jacobi method to the case of skew-symmetric matrices by employing the Quaternion rotation instead of the two-dimensional rotation of the Jacobi method. Goldstine and Horwitz in [2] have extended the Jacobi method to normal matrices by plane unitary transformations. For a non-normal matrix, it is not possible to use unitary transformations alone [1]. For general matrices, Ruhe in [8] extended the Jacobi method to general matrices by unitary transformations and plane shears. The Jacobi-Davidson method [9] was devised to obtain a few eigenpairs for large sparse matrices.

Henrici [5] proposed the direct extension of the Jacobi method to Hermitian matrices and showed the quadratic convergence rate of his extended method. His method used complex arithmetics in computing. We introduce a new extended Jacobi method for Hermitian matrices without using complex arithmectics. Our method constructs the real symmetric matrices augmented from Hermitian matrices,

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and apply a specially designed Jacobi method to the augmented matrices, which we call an *augmented Jacobi method*. Our method is doing only real arithmetics. We also note that the presented method is readily applicable to skew-Hermitian and real skew-symmetric matrices, since the multiplication by $i = \sqrt{-1}$ to skew-Hermitian or real skew-symmetric matrices results in Hermitian matrices.

2. Brief Review of the Jacobi Method

The Jacobi method [6] is an efficient tool for finding the eigensystem of real symmetric matrices. We summarize it in this section.

Definition For a square matrix A, we declare the following norms.

$$\begin{aligned} \|A\|_{Fr} &= \sqrt{\sum_{i,j} (a_{ij})^2} \\ \|A\|_{Off} &= \sqrt{\sum_{i\neq j} (a_{ij})^2} \\ \|A\|_{Diag} &= \sqrt{\sum_{i} (a_{ii})^2} \end{aligned}$$

The Off norm measures how much the matrix is close to a diagonal matrix.

Lemma 2.1. *If P is an orthgonal matrix, then $\|A\|_{Fr} = \left\|P^TAP\right\|_{Fr}$ for any square matrix A of the same size as P.*

Proof. First note that $\|A\|_{Fr}^2 = tr\left(A^TA\right)$, then the argument is clear from

$$\left\|P^TAP\right\|_{Fr}^2 = tr\left(\left(P^TAP\right)^T\left(P^TAP\right)\right) = tr\left(P^TA^TAP\right) = tr\left(A^TA\right).$$

□

From $\|A\|_{Fr} = \left\|P^TAP\right\|_{Fr}$ and $\|A\|_{Fr}^2 = \|A\|_{Off}^2 + \|A\|_{Diag}^2$, we have the equivalence relation $\left\|P^TAP\right\|_{Off} < \|A\|_{Off}$ if and only if $\left\|P^TAP\right\|_{Diag} > \|A\|_{Diag}$.

Consider a symmetric matrix A, and assume an element $a_{pq} \neq 0$ with $p \neq q$. Jacobi considered the following orthogonal matrix P whose similarity transformation can efficiently eliminate the element.

$$\begin{aligned} P_{pp} &= \cos\theta \\ P_{pq} &= \sin\theta \\ P_{qp} &= -\sin\theta \end{aligned} \tag{1}$$

$$P_{qq} = \quad \cos\theta$$
$$P_{ij} = \delta_{ij} \text{ if } i \neq p, q \text{ or } j \neq p, q$$

for some angle ϕ. Using this orthogonal matrix, we apply a similarity transformation $A' = P^T AP$. Then A' is symmetric and has the same elements as A except the p^{th} and q^{th} row vectors and the p^{th} and q^{th} column vectors as follows.

$$\begin{aligned}
&A'_{pp} = \cos^2\theta A_{pp} - 2\sin\theta\cos\theta A_{pq} + \sin^2\theta A_{qq} \\
&A'_{qq} = \cos^2\theta A_{qq} + 2\sin\theta\cos\theta A_{pq} + \sin^2\theta A_{pp} \\
&A'_{pq} = A'_{qp} = (\cos^2\theta - \sin^2\theta)A_{pq} + \sin\theta\cos\theta(A_{pp} - A_{qq}) \\
&A'_{ip} = A'_{pi} = \cos\theta A_{pi} - \sin\theta A_{qi}, && \text{if } i \neq p, q \\
&A'_{iq} = A'_{qi} = \cos\theta A_{iq} + \sin\theta A_{ip}, && \text{if } i \neq p, q \\
&A'_{ij} = A_{ij}, && \text{if } i, j \neq p, q.
\end{aligned} \tag{2}$$

Since the similarity transformation preserves the eigenvalues and changes the eigenvectors by a multiplication of P^T, we can calculate the eigensystem of A from the eigensystem of A'. To make the new matrix A' closer to diagonal matrix, we choose θ to set $A'_{pq} = 0$, or $\cos(2\theta)A_{pq} + \sin(2\theta)\frac{A_{pp}-A_{qq}}{2} = 0$. We briefly review the well known theorem below, that will be extended in the next section.

Proposition 2.2. *With the orthogonal matrix P in equation 1, the new matrix A' is more diagonal than A in the sense that*

$$\|A'\|^2_{Off} = \|A\|^2_{Off} - 2\,(a_{pq})^2\,.$$

Proof. By the lemma 2.1, we have $\|A'\|^2_{Fr} = \|A\|^2_{Fr}$. Using the relations $\|A'\|^2_{Fr} = \|A'\|^2_{Off} + \|A'\|^2_{Diag}$ and $\|A\|^2_{Fr} = \|A\|^2_{Off} + \|A\|^2_{Diag}$, we instead show that $\|A'\|^2_{Diag} = \|A\|^2_{Diag} + 2\,(a_{pq})^2$. The diagonal elements of A' are the same as those of A except the p^{th} and q^{th} as shown in equation 2. The updates of the two diagonal elements can be formulated in the following 2×2 matrix equation.

$$\begin{pmatrix} a'_{pp} & a'_{pq} \\ a'_{qp} & a'_{qq} \end{pmatrix} = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} a_{pp} & a_{pq} \\ a_{qp} & a_{qq} \end{pmatrix} \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix}$$

Applying lemma 2.1 to the above equation, we have $\left(a'_{pp}\right)^2 + 2\left(a'_{pq}\right)^2 + \left(a'_{qq}\right)^2 = (a_{pp})^2 + 2\,(a_{pq})^2 + (a_{qq})^2$. The angle θ was chosen to make $a'_{pq} = 0$, so that $\left(a'_{pp}\right)^2 + \left(a'_{qq}\right)^2 = (a_{pp})^2 + 2\,(a_{pq})^2 + (a_{qq})^2$. Now we have $\|A'\|^2_{Diag} = \|A\|^2_{Diag} + 2\,(a_{pq})^2$ that comples the proof. $\square$

There are some discussions which element $a_{pq} \neq 0$ to be chosen, [reduced cyclic]. The best option in decreasing the Off norm is to select the largest one, i.e.

$$|a_{pq}| = \max_{i \neq j} |a_{ij}| .$$

Proposition 2.3. *Assume that the Jacobi method is sequentially applied to an $N \times N$ symmetric matrix A with the maximum choice. Let $A^{(n)}$ be the n^{th} stage, then, for each $n = 0, 1, 2, \cdots$,*

$$\left\| A^{(n)} \right\|_{Off}^2 \leq \|A\|_{Off}^2 \left(1 - \frac{2}{N^2 - N}\right)^n .$$

Proof. Let $\left|a_{pq}^{(n)}\right| = \max_{i \neq j} \left|a_{ij}^{(n)}\right|$, then $\|A^{(n)}\|_{Off}^2 \leq \left|a_{pq}^{(n)}\right|^2 \left(N^2 - N\right)$. Since

$$\left\| A^{(n+1)} \right\|_{Off}^2 = \left\| A^{(n)} \right\|_{Off}^2 - 2\left|a_{pq}^{(n)}\right| \leq \left\| A^{(n)} \right\|_{Off}^2 \left(1 - \frac{2}{N^2 - N}\right)$$

for each n, we have the above inequality. □

3. METHOD 1 : CLASSICAL JACOBI METHOD ON THE AUGMENTED MATRIX

Consider a Hermitian matrix $H = A + iB$, where A and B are real matrices. We denote by $\tilde{H}$ the following augmented matrix:

$$\tilde{H} = \begin{pmatrix} A & -B \\ B & A \end{pmatrix}$$

When H is an $n \times n$ Hermitian matrix, $\tilde{H}$ is a $2n \times 2n$ real symmetric matrix. Let λ be an eigenvalue of the Hermitian matrix H with its corresponding eigenvector $u + iv$, where u and v are real column vectors, then we have

$$(A + iB)(u + iv) = \lambda(u + iv) \quad \Leftrightarrow \quad \begin{pmatrix} A & -B \\ B & A \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix} = \lambda \begin{pmatrix} u \\ v \end{pmatrix} .$$

This shows that the eigensystems of H and $\tilde{H}$ are closely related:

- λ is an eigenvalue of H if and only if it is an eigenvalue of $\tilde{H}$.
- Associated with the same eigenvalue λ, $u + iv$ is an eigenvector of H if and only if $\left(\begin{smallmatrix} u \\ v \end{smallmatrix}\right)$ is an eigenvector of $\tilde{H}$.
- Associated with the same eigenvalue λ, $\left(\begin{smallmatrix} u \\ v \end{smallmatrix}\right)$ is an eigenvector of $\tilde{H}$ if and only if $\left(\begin{smallmatrix} -v \\ u \end{smallmatrix}\right)$ is an eigenvector of $\tilde{H}$.

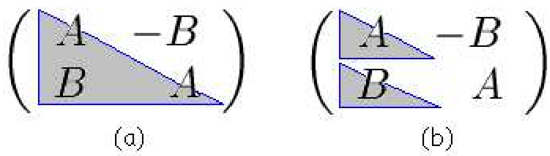

Figure 1. Computational supports of the Direct Jacobi Method (a) and the Augmented Jacobi Method (b) applied to the augmented real symmetric matrix

In particular, each eigenvector of H is repeated twice in $\tilde{H}$. Since $\tilde{H}$ is real and symmetric, its eigenvalues and eigenvectors can be computed by the Jacobi method in Section 2, and the eigenvalues and eigenvectors of H can be obtained through the above relation between them. This direct approach of the Jacobi method, which we call the *direct Jacobi method*, treats the matrix $\tilde{H}$ as a real symmetric method, and it updates the half of its elements as depicted in Figure 1(a). In the next section, we introduce a new Jacobi method that keeps the block structure of the matrix $\tilde{H}$, and hence it updates only the elements of the shaded region in Figure 1(b).

We apply the Jacobi method on the real symmetric matrix $\tilde{H}$. Example shows the first update of the matrix. Note that the block structure of $\tilde{H}$ was broken. Note that the number of elements updated is $4N$: since $\tilde{H}$ is symmetric, only the upper triangular elements need be updated.

Proposition 3.1. *Let H be a Hermitian matrix of $N \times N$. Let the method 1 is operated on the real symmetric matrix $\tilde{H}$, then*

$$\left\|\tilde{H}^{(n)}\right\|_{Off}^{2} \leq \left\|\tilde{H}\right\|_{Off}^{2} \left(1 - \frac{1}{2N^2 - N}\right)^{n}.$$

Proof. Obvious □

Note on Skew-Hermitian Matrices

Consider an $n \times n$ skew-Hermitian matrix $S = A + iB$, where A and B are real matrices. From the property of the skew-symmetry, $A^T = -A$ and $B^T = B$. Let $i\lambda$ be an eigenvalue of the skew-Hermitian matrix S with its corresponding eigenvector $u + iv$, where u and v are real column vectors, then we have

$$(A + iB)(u + iv) = i\lambda(u + iv) \quad \Leftrightarrow \quad \begin{pmatrix} B & A \\ -A & B \end{pmatrix} \begin{pmatrix} -v \\ u \end{pmatrix} = \lambda \begin{pmatrix} -v \\ u \end{pmatrix}.$$

We denote the $2n \times 2n$ real symmetric matrix on the right hand side by $\tilde{S}$. In the similar way to the case of Hermitian matrices, the eigensystems of S and $\tilde{S}$ are closely related. as follows.

- $i\lambda$ is an eigenvalue of S if and only if λ is an eigenvalue of $\tilde{S}$.
- $i\lambda$ and $u + iv$ is an eigenpair of S if and only if λ and $\binom{-v}{u}$ is an eigenpair of $\tilde{S}$.
- Associated with the same eigenvalue λ, $\binom{-v}{u}$ is an eigenvector of $\tilde{S}$ if and only if $\binom{u}{v}$ is an eigenvector of $\tilde{S}$.

Note that the block structure of $\tilde{S}$ is the same as $\tilde{H}$, and thus the augmented Jacobi method is also applicable to $\tilde{S}$. This is not surprising since the multiplication by $i = \sqrt{-1}$ to skew-Hermitian matrices results in Hermitian matrices.

4. METHOD 2 : A NEW JACOBI PRESERVING THE SYMMETRY

Method 1 broke the block symmetry structure of the augmented matrix. In this section, we show a simple fix-up that can preserve the symmetry that will bring a big saving in memory and speed. When $\left|\tilde{h}_{pq}\right| = \max_{i \neq j} \left|\tilde{h}_{ij}\right|$, there are two cases. For each case we show that we can fix the symmetry. We modify the Jacobi method in Section 2 to keep the block structure of $\tilde{H}$ so that we can reduce the half of the operation counts and save memory space. Assume a $2n \times 2n$ real symmetric matrix $\tilde{H}$,

$$\tilde{H} = \begin{pmatrix} A & -B \\ B & A \end{pmatrix}$$

with $A = A^T$ and $B = -B^T$. Note that the augmented matrix $\tilde{H}$ has the block structure:

- The two diagonal blocks are the same.
- The two off-diagonal blocks are the negative of each other.
- The diagonal blocks are symmetric.
- The off-diagonal blocks are skew-symmetric.

As in the Jacobi Method, we introduce a similarity transformation that reduces the Off norm. If $\tilde{H}$ is not diagonal, there are two possible cases: either $A_{pq} \neq 0$ or $B_{pq} \neq 0$ for some $p \neq q$. In either case the similarity transformation keeps the block structure of the augmented matrix, and the computational support of this algorithm can be reduced to the half compared to the direct Jacobi method as depicted in Figure 1.

4.1. Case $B_{pq} \neq 0$. Suppose $B_{pq} \neq 0$ with $1 \leq p, q \leq n$. Note that $p \neq q$ since B is skew-symmetric. We define an orthogonal matrix $\tilde{P}$ as follows

$$\tilde{P} = \begin{pmatrix} Q & R \\ -R & Q \end{pmatrix}$$

$$\begin{cases} Q_{pp} & = \cos\theta \\ Q_{qq} & = \cos\theta \\ Q_{ij} & = \delta_{ij} \text{ otherwise} \end{cases} \quad \begin{cases} R_{pq} & = \sin\theta \\ R_{qp} & = \sin\theta \\ R_{ij} & = 0 \text{ otherwise} \end{cases}$$

Note that Q is diagonal and R is symmetric. We do a similarity transformation $\tilde{H}' = \tilde{P}^T \tilde{H} \tilde{P}$. Written in block structure $\tilde{H}' = \begin{pmatrix} A' & -B' \\ -B'^T & C' \end{pmatrix}$, the block elements are

$$A' = C' = QAQ - RBQ + QBR + RAR$$
$$B' = -B'^T = -QAR + RBR + QBQ + RAQ.$$

Note that $\tilde{H}' = \begin{pmatrix} A' & -B' \\ B' & A' \end{pmatrix}$ is again of the same block structure as $\tilde{H}$.

4.2. Case $A_{pq} \neq 0$. Suppose $A_{pq} \neq 0$ with $1 \leq p, q \leq n$. We define an orthogonal matrix $\tilde{P}$ as follows

$$\tilde{P} = \begin{pmatrix} Q & 0 \\ 0 & Q \end{pmatrix}$$

$$\begin{cases} Q_{pp} & = \cos\theta \\ Q_{qq} & = \cos\theta \\ Q_{pq} & = \sin\theta \\ Q_{qp} & = -\sin\theta \\ Q_{ij} & = \delta_{ij} \text{ otherwise} \end{cases}$$

Using the above orthogonal matrix, we do a similarity transformation $\tilde{H}' = \tilde{P}^T \tilde{H} \tilde{P}$. Written in block structure $\tilde{H}' = \begin{pmatrix} A' & -B' \\ -B'^T & C' \end{pmatrix}$, the block elements are

$$A' = C' = Q^T A Q$$
$$B' = -B'^T = Q^T B Q.$$

Note that $\tilde{H}' = \begin{pmatrix} A' & -B' \\ B' & A' \end{pmatrix}$ is again of the same block structure as $\tilde{H}$.

4.3. Decreasing property of the Off norm. In this subsection, we show that the similarity transformation reduces the Off norm so that the successive application of the similarity transformation to the augmented matrix converges to a diagonal matrix.

Proposition 4.1. *Under the notations and hypotheses in this section, if θ is chosen as in Section 2 so that $\tilde{H}'_{rs} = 0$ for $1 \le r, s \le 2n$ with $r \neq s$,*

$$\|\tilde{H}'\|^2_{Off} = \|\tilde{H}\|^2_{Off} - 4\tilde{H}^2_{rs}.$$

Proof. Note that Frobenius norm does not change under a similarity transformation, and that the Off norm of a real symmetric matrix is the substraction of its Frobenius norm by the sum of the squares of its diagonal elements. Thus, $\|\tilde{H}'\|_F = \|\tilde{H}\|_F$, where $\|\cdot\|_F$ denotes Frobenius norm, and

$$\|\tilde{H}'\|^2_{\mathrm{Off}} = \|\tilde{H}'\|^2_{\mathrm{F}} - 2\sum_i A'^2_{ii} = \|\tilde{H}\|^2_{\mathrm{F}} - 2\sum_i A'^2_{ii} = \|\tilde{H}\|^2_{\mathrm{Off}} + 2\sum_i \left(A^2_{ii} - A'^2_{ii}\right)$$

Thus, we only need to show $\sum_i \left(A^2_{ii} - A'^2_{ii}\right) = -2\tilde{H}^2_{r,s}$.

There are two cases: either $\tilde{H}'_{rs} = A'_{pq}$ or $\tilde{H}'_{rs} = B'_{pq}$ for $1 \le p, q \le n$. First, assume that $\tilde{H}'_{rs} = A'_{pq}$. In this case A' is $Q^T A Q$ and has the same elements as appeared in Section 2. An easy calculation shows $A'^2_{pp} + A'^2_{qq} = A^2_{pp} + A^2_{qq} + 2A^2_{pq}$ and $A'_{ii} = A_{ii}$ for $i \neq p, q$. Thus

$$\sum_i \left(A^2_{ii} - A'^2_{ii}\right) = A^2_{pp} + A^2_{qq} - A'^2_{pp} - A'^2_{qq} = -2A^2_{pq} = -2\tilde{H}^2_{rs}.$$

We now assume that $\tilde{H}'_{rs} = B'_{pq}$. Then

$$\begin{aligned} A'_{pp} &= \cos^2\theta A_{pp} + 2\sin\theta\cos\theta B_{pq} + \sin^2\theta A_{qq} \\ A'_{qq} &= \cos^2\theta A_{qq} - 2\sin\theta\cos\theta B_{pq} + \sin^2\theta A_{pp} \\ A'_{ii} &= A_{ii} \quad \text{if } i \neq p, q. \end{aligned}$$

and A'_{ii} has the same formula as the previous case except A_{pq} replaced by $-B_{pq}$. Thus the same calculation as the previous case shows that $\sum_i \left(A^2_{ii} - A'^2_{ii}\right) = -2B^2_{pq} = -2\tilde{H}^2_{rs}$. This completes the proof. □

Proposition 4.2. *Let H be a Hermitian matrix of $N \times N$. Let the method 2 be operated on the real symmetric matrix $\tilde{H}$, then*

$$\left\|\tilde{H}^{(n)}\right\|^2_{Off} \le \left\|\tilde{H}\right\|^2_{Off} \left(1 - \frac{1}{N^2 - N}\right)^n.$$

Proof. $\tilde{H}$ has $4N^2 - 2N$ number of off diagonal elements. Since the method preserves the block-symmetry structure, the diagonal elements in the upper-right and lower-bottom blocks keeps zero throughout the iteration. Therefore $\left\|\tilde{H}^{(n)}\right\|_{Off}^2 \leq \left(\tilde{H}_{rs}\right)^2 \left(\left(4N^2 - 2N\right) - 2N\right)$ for $\left|\tilde{H}_{rs}\right| = \max_{i\neq j}\left|\tilde{H}_{ij}^{(n)}\right|$. From the above propoosition $\left\|\tilde{H}^{(n+1)}\right\|_{Off}^2 \leq \left\|\tilde{H}^{(n)}\right\|_{Off}^2 \left(1 - \frac{1}{N^2-N}\right)$, and follows the inequaality . □

A note on the block structure of eigenvector matrix. We sequentially construct eigenvalue matrix $\tilde{D}$ and eigenvector matrix $\tilde{V}$ as follows: Starting from $\tilde{D} := \tilde{H}$ and $\tilde{V} := I$, find the largest off-diagonal element $\tilde{D}_{pq}$ of $\tilde{D}$ in magnitude and then apply the similarity transformation to update $\tilde{D} := \tilde{P}^T\tilde{D}\tilde{P}$ and $\tilde{V} := \tilde{V}\tilde{P}$ until $\tilde{D}$ becomes diagonal. Note that $\tilde{V}$ has the same block structure as $\tilde{H}$, and hence only its half elements need to be stored and updated.

5. Example

5.1. Example of Hermitian matrix. Consider an $N \times N$ Hermitian matrix H whose elements are given by $H_{ij} = \left((i+j)^2 + \mathbf{i}\,(i-j)^3\right)$. When $N = 3$, H and its associated real symmetric matrix $\tilde{H}$ are as follows.

$$H = \begin{pmatrix} 4 & 9-\mathbf{i} & 16-8\mathbf{i} \\ 9+\mathbf{i} & 16 & 25-\mathbf{i} \\ 16+\mathbf{i} & 25+\mathbf{i} & 36 \end{pmatrix}, \quad \tilde{H} = \begin{pmatrix} 4 & 9 & 16 & 0 & 1 & 0 \\ 9 & 16 & 25 & -1 & 0 & 1 \\ 16 & 25 & 36 & 0 & -1 & 0 \\ 0 & -1 & 0 & 4 & 9 & 16 \\ 1 & 0 & -1 & 9 & 16 & 25 \\ 0 & 1 & 0 & 16 & 25 & 36 \end{pmatrix}$$

Note that $\tilde{H}_{23} = 25$ is the maximum in absolute value among the off-diagonal elements of $\tilde{H}$. The classic Jacobi method and the block-symmetry Jacobi eliminate the element in the following ways.

$$\tilde{H}^{(1)} = \begin{pmatrix} 4.000 & 18.295 & 1.517 & -0.000 & 1.000 & 8.000 \\ 18.295 & 52.926 & 0.000 & -7.185 & -0.828 & 0.561 \\ 1.517 & 0.000 & \text{-0.926} & -3.657 & -0.561 & -0.828 \\ \text{-0.000} & \text{-7.185} & \text{-3.657} & 4.000 & 9.000 & 16.000 \\ 1.000 & \text{-0.828} & \text{-0.561} & 9.000 & 16.000 & 25.000 \\ 8.000 & 0.561 & \text{-0.828} & 16.000 & 25.000 & 36.000 \end{pmatrix} \text{(classic Jacobi)}$$

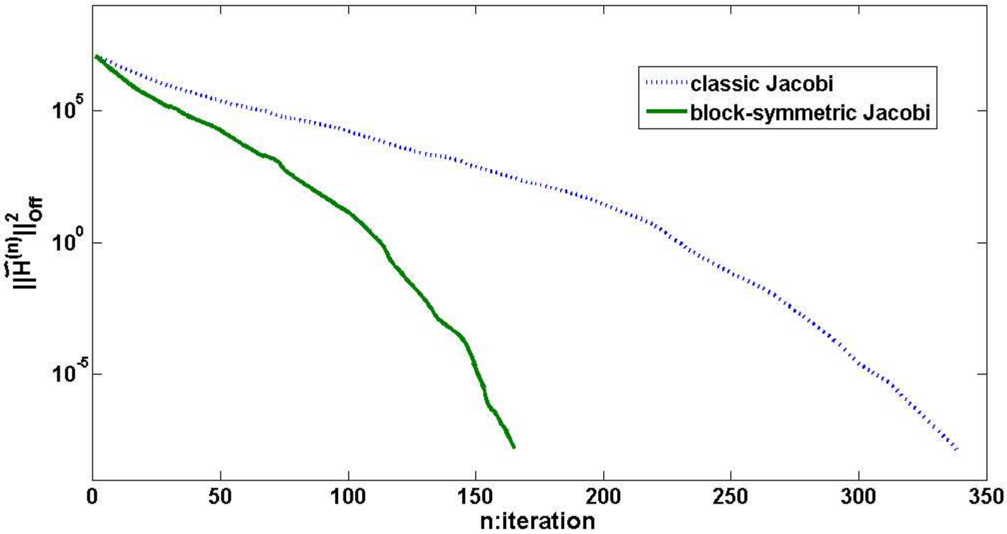

Figure 2. Convergences of the Jacobi methods for the Hermitian matrix H with $N = 10$

$$\tilde{H}^{(1)} = \begin{pmatrix} 4.000 & 18.295 & 1.517 & 0 & 7.185 & 3.657 \\ 18.295 & 52.926 & 0.000 & 7.185 & 0 & -1.000 \\ 1.517 & 0.000 & -0.926 & 3.657 & -1.000 & 0 \\ 0 & -7.185 & -3.657 & 4.000 & 18.295 & 1.517 \\ -7.185 & 0 & 1.000 & 18.295 & 52.926 & 0.000 \\ -3.657 & 1.000 & 0 & 1.517 & 0.000 & -0.926 \end{pmatrix} \begin{pmatrix} \text{block-} \\ \text{-symmetric} \\ \text{Jacobi} \end{pmatrix}$$

Using the symmetric structures, only the shaded elements are stored and updated. For an $N \times N$ Hermitian matrix, the classic Jacobi method is required to store $2N^2 + N$ number of elements and to update $4N$ number of elements in one step. On the other hand, the block-symmetric Jacobi method is required to store N^2 number of elements and to update $4N$ number of elements in one step. Proposition 3.1 and 4.2 show that the block-symmetric Jacobi method converges faster than the classic Jacobi. Figure 2 compares the two methods in decreasing the Off norms, and confirms the expectation of the propositions. Until the convergence of the Off norm within a machine precision 10^{-8}, the block-symmetric Jacobi method took only a half number of iterations compared with the classic Jacobi. Recalling that the same number of elements are updated in both methods, we observe that the block-symmetric Jacobi method consumes a half times less memory and performs twice faster than the classic Jacobi.

5.2. Example of skew-Hermitian matrix. Consider an $N \times N$ skew-Hermitian matrix S with $S_{ij} = \left(\sin(i-j) + \mathbf{i}\frac{1}{i+j-1}\right)$ for each i and j. When $N = 3$, S and its associated real symmetric matrix $\tilde{S}$ are as follows.

$$S = \begin{pmatrix} 0.00 + \mathbf{i}\cdot 1.00 & -0.84 + \mathbf{i}\cdot 0.50 & -0.91 + \mathbf{i}\cdot 0.33 \\ 0.84 + \mathbf{i}\cdot 0.50 & 0.00 + \mathbf{i}\cdot 0.33 & -0.84 + \mathbf{i}\cdot 0.25 \\ 0.91 + \mathbf{i}\cdot 0.33 & 0.84 + \mathbf{i}\cdot 0.25 & 0.00 + \mathbf{i}\cdot 0.20 \end{pmatrix}$$

$$\tilde{S} = \begin{pmatrix} -1.00 & -0.50 & -0.33 & 0.00 & -0.84 & -0.91 \\ -0.50 & -0.33 & -0.25 & 0.84 & 0.00 & -0.84 \\ -0.33 & -0.25 & -0.20 & 0.91 & 0.84 & 0.00 \\ -0.00 & 0.84 & 0.91 & -1.00 & -0.50 & -0.33 \\ -0.84 & -0.00 & 0.84 & -0.50 & -0.33 & -0.25 \\ -0.91 & -0.84 & -0.00 & -0.33 & -0.25 & -0.20 \end{pmatrix}$$

Note that $\left|\tilde{S}_{34}\right|$ is the maximum among the off-diagonal elements of $\tilde{S}$. Eliminating the element, the classic Jacobi method and the block-symmetric Jacobi method result in the followings.

$$\tilde{S}^{(1)} = \begin{pmatrix} 0.393 & 0.431 & -0.182 & 0.279 & -0.251 & -0.000 \\ 0.431 & -0.333 & -0.250 & 0.841 & 0.000 & -0.879 \\ -0.182 & -0.250 & -0.200 & 0.909 & 0.841 & -0.279 \\ 0.279 & 0.841 & 0.909 & -1.000 & -0.500 & -0.182 \\ -0.251 & 0.000 & 0.841 & -0.500 & -0.333 & -0.841 \\ -0.000 & -0.879 & -0.279 & -0.182 & -0.841 & -1.593 \end{pmatrix} \text{(classic Jacobi)}$$

$$\tilde{S}^{(1)} = \begin{pmatrix} -0.393 & -0.431 & 0.333 & 0.000 & -0.251 & 0.000 \\ -0.431 & 0.333 & 0.841 & 0.251 & 0.000 & -0.879 \\ 0.333 & 0.841 & 1.593 & -0.000 & 0.879 & 0.000 \\ 0.000 & 0.251 & -0.000 & -0.393 & -0.431 & 0.333 \\ -0.251 & 0.000 & 0.879 & -0.431 & 0.333 & 0.841 \\ 0.000 & -0.879 & 0.000 & 0.333 & 0.841 & 1.593 \end{pmatrix} \left(\begin{array}{c}\text{block-} \\ \text{-symmetric} \\ \text{Jacobi}\end{array}\right)$$

Same as in the previous example, only the shaded elements are stored and taken care of. For an $N \times N$ skew-Hermitian matrix, the classic Jacobi method is required to store $2N^2 + N$ number of elements and to update $4N$ number of elements in one step. On the other hand, the block-symmetric Jacobi method is required to store N^2 number of elements and to update $4N$ number of elements in one step. Figure 3 compares the two methods in decreasing the Off norms, and confirms the expectation of the propositions 3.1 and 4.2. Until the convergence of the Off norm within a machine precision 10^{-8}, the block-symmetric Jacobi method took only a half number of iterations compared with the classic Jacobi. Recalling that the

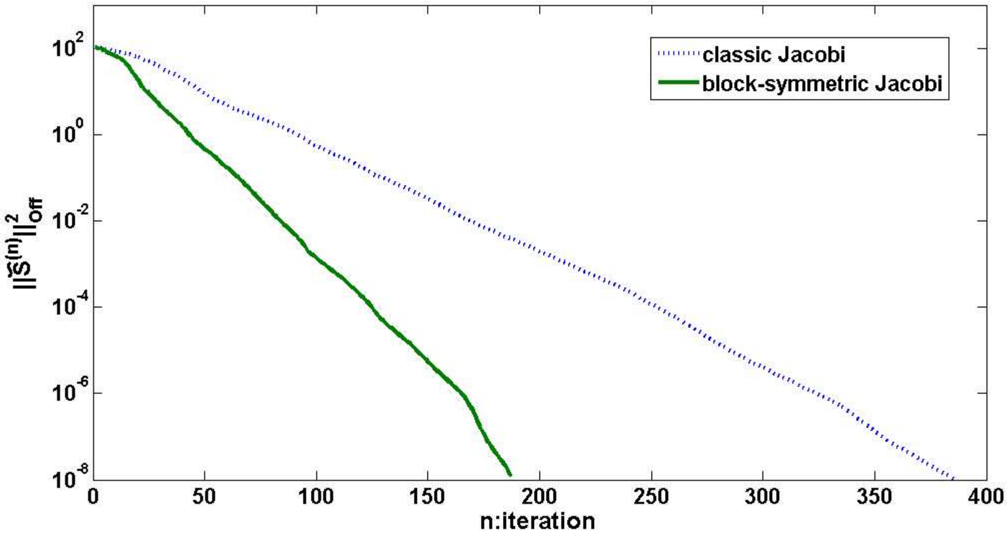

Figure 3. Convergences of the Jacobi methods for the skew-Hermitian matrix S with $N = 10$

same number of elements are updated in both methods, we observe that the block-symmetric Jacobi method consumes a half times less memory and performs twice faster than the classic Jacobi.

5.3. Example of matrix with repeating eigenvalues. If a Hermitian matrix has distinct eigenvalues, each eigenvector appears once again after multiplied by i in the augmented matrix and any of the repeated can be chosen safely. However, the safe choice is not guaranteed any more in the presence of eigenvalue having multiplicity. Consider the following Hermitian matrix having eigenvalues 2 and -1.

$$\begin{pmatrix} 1 & 1 & i \\ 1 & 1 & -i \\ -i & i & 1 \end{pmatrix}$$

The Jacobi method directly applied to the augmented matrix as in Section 3 produces the eigenvalue matrix $\tilde{D}$ and eigenvector matrix $\tilde{V}$ as appeared below. The decimal points after the fourth were skipped.

$$\tilde{D} = \begin{pmatrix} 2.000 & 0.000 & 0.000 & 0.000 & 0.000 & 0.000 \\ 0.000 & 2.000 & 0.000 & 0.000 & 0.000 & 0.000 \\ 0.000 & 0.000 & 2.000 & 0.000 & 0.000 & 0.000 \\ 0.000 & 0.000 & 0.000 & 2.000 & 0.000 & 0.000 \\ 0.000 & 0.000 & 0.000 & 0.000 & -1.000 & 0.000 \\ 0.000 & 0.000 & 0.000 & 0.000 & 0.000 & -1.000 \end{pmatrix}$$

$$\tilde{V} = \begin{pmatrix} 0.707 & 0.000 & -0.408 & 0.000 & 0.000 & 0.577 \\ 0.707 & 0.000 & 0.408 & 0.000 & 0.000 & -0.577 \\ 0.000 & 0.707 & 0.000 & -0.408 & 0.577 & 0.000 \\ 0.000 & 0.707 & 0.000 & 0.408 & -0.577 & 0.000 \\ 0.000 & 0.000 & 0.000 & 0.816 & 0.577 & 0.000 \\ 0.000 & 0.000 & 0.816 & 0.000 & 0.000 & 0.577 \end{pmatrix}$$

Associated with eigenvalue 2, the above results read that we need to select two linearly independent vectors from the four vectors coming from the first four column vectors of $\tilde{V}$.

$$\begin{pmatrix} 0.707 \\ 0.707 \\ 0 \end{pmatrix}, \begin{pmatrix} 0.707i \\ 0 \\ 0.707 \end{pmatrix}, \begin{pmatrix} -0.408 \\ 0.408 \\ 0.816i \end{pmatrix}, \begin{pmatrix} 0.408i \\ 0.816i \\ -0.408 \end{pmatrix}$$

In the above case, the first and the third one should be chosen to keep the orthogonality between eigenvectors.

If we do the same as above for a diagonal matrix with diagonal elements 0, 0 and 1, the direct Jacobi method stops at no step and after the sorting, the first and the second columns should be chosen as eigenvectors out of the four vectors. Thus after the computation of the direct approach, the existence of any repeating eigenvalues should be checked, and the selection process of eigenvectors should be also accompanied.

On the other hand, the augmented Jacobi method keeps the block structure and we are free from the above selection process: we can just safely take the first half block. For the same matrix, the augmented Jacobi method produces the following results.

$$\tilde{D} = \begin{pmatrix} 2.000 & 0.000 & 0.000 & -0.000 & -0.000 & -0.000 \\ 0.000 & 2.000 & 0.000 & 0.000 & -0.000 & -0.000 \\ 0.000 & 0.000 & -1.000 & 0.000 & 0.000 & -0.000 \\ 0.000 & 0.000 & 0.000 & 2.000 & 0.000 & 0.000 \\ -0.000 & 0.000 & 0.000 & 0.000 & 2.000 & 0.000 \\ -0.000 & -0.000 & 0.000 & 0.000 & 0.000 & -1.000 \end{pmatrix}$$

$$\tilde{V} = \begin{pmatrix} 0.707 & 0.000 & -0.577 & -0.000 & -0.408 & -0.000 \\ 0.707 & 0.000 & 0.577 & -0.000 & 0.408 & -0.000 \\ 0.000 & 0.816 & 0.000 & -0.000 & -0.000 & 0.577 \\ 0.000 & 0.408 & 0.000 & 0.707 & 0.000 & -0.577 \\ 0.000 & -0.408 & 0.000 & 0.707 & 0.000 & 0.577 \\ 0.000 & 0.000 & -0.577 & 0.000 & 0.816 & 0.000 \end{pmatrix}$$

Associated with eigenvalue 2, the first and second column vectors of $\tilde{V}$ are automatically orthogonal and can be safely chosen as eigenvectors.

Also for skew-Hermitian matrices, with the same reason, the augmented Jacobi method is free from the comparison of eigenvalues and selection process of eigenvectors that might be necessary to the direct Jacobi method.

6. Conclusion

In this work, a new extended Jacobi method has been developed for computing eigenvalues and eigenvectors of Hermitian matrices. This method does not use any complex arithmetics, while a known Jacobi-like method for Hermitian matrices does. It can also be easily applied to skew-Hermitian and real skew-symmetric matrices just by switching blocks of augmented matrices. It is computationally efficient in choosing eigenvectors and works for any Hermitian matrices.

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