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PARALLEL NUMERICAL ALGORITHM FOR SPECTRAL PROBLEM OF BLOCK HERMITIAN MATRICES

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ABSTRACT. An effective parallel numerical algorithm for solving the complete spectral problem for an arbitrary block Hermitian matrix is proposed. It is modification of Jacobi's cyclic method [4] and a generalization of the parallel modification of the Jacobi's method, proposed by Sameh (1971).

1. A description of the algorithm. Let $A = A_{ij}$ be $n \times n$ a Hermitian block matrix with square blocks A_{ij} of order b. Thus A is a scalar square matrix of order nb. The algorithm suggested in the present paper is reduced to the construction of the following sequence of matrices, similarly to Jacoby's classical method

$$A^{(0)} = A,\ A^{(1)},\ A^{(2)}, \dots , \tag{1}$$

where each matrics $A^{(\nu+1)}$ is obtained from the previous one $A^{(\nu)}$ by unitary similar transformation of the type

$$A^{(v+1)} = U^{(v)H} A^{(v)} U^{(v)} , \qquad (U^{(v)H} U^{(v)} = I) . \tag{2}$$

We shall give an idea for the algorithm by describing its first step, which is as follows:

$$\tilde{A} = U^H A U , \tag{3}$$

where the unitary matrix

$$U = (U_{ij}) = \textstyle\prod_{k=1}^{n} U_k \qquad \text{if } n \text{ is odd and}$$

$$U = (U_{ij}) = \textstyle\prod_{k=0}^{n} U_k \qquad \text{if } n \text{ is even.}$$

Each U_k is a product of α_k unitary matrices $U_{k_1}, U_{k_2}, \dots, U_{k_\alpha}$ and $\alpha_k = b^2$ or $\alpha_k = (b^2 - b)/2$. As we shall see below each U_{kp} consists exactly of n or $4[n/2]$ or $4[n/2] + 1$

non-zero blocks, where $[x]$ is the greatest integer less than or equal to x. The first two cases hold for even n. The last one is valid for an odd n. Moreover, if there exist n non-zero blocks, then they are on the main diagonal of U_{kp}.

Let each $\gamma = 2[n/2]+1$ consequtive unitary transformation of a given matrix A with matrices U_k be denoted by a sweep. Let $A_{k+1} = U_k^H A_k U_k$. If n is an even number, then $k = 0, 1, \ldots, n$ and $A_0 = A^{(0)}$, $A^{(1)} = A_{n+1}$. If n is an odd number, then $k = 1, 2, \ldots, n$ and $A_1 = A^{(0)}$, $A^{(1)} = A_{n+1}$ and

$$U_k = U_{k1} U_{k2} \ldots U_{k\alpha_k} \ . \tag{4}$$

It is typical for the presented algorithm that each unitary matrix U_{kp} annihilates exactly one element in exactly $[(n+1)/2]$ or $[n/2]$ different blocks of the matrices $V^H A_k V$ and $V = \prod_\mu^p U_{k\mu}$. Let us denote by I_k and J_k the sets of the values od the first and second indices of the blocks of matrices A_k ($0 \le s \le k$ or $1 \le s \le k$) whose elements have been annihilated so far. A_{k+1} is obtained by unitary transformations with matrices of type U_{kp} ($1 \le p \le \alpha_k$). For each p and fixed k the localisations of the non-zero (zero) blocks in U_{kp} are not changed. These non-zero block are arranged in such a way that the elements in blocks (i,j) from $V^H A_k V$ for which $i \notin I_k$ and $j \notin J_k$ to be annihilated. Moreover, the positions of these elements in a given block change cyclicly.

We want to construct the matrix $U_{kp} = \{U_{ij}(k,p)\}$ so that the element being in position (l,q) of an (r,s)-block of $V^H A_k V$ annihilates.

Let for $r \neq s$

$$\begin{aligned} U_{rr}(k,p) &= \mathrm{diag}\,[I_{l-1},\ \cos(\varphi),\ I_{b-l}]\ , \\ U_{ss}(k,p) &= P_{lq} U_{rr}(k,p) P_{l,q}\ , \\ U_{rs}(k,p) &= \begin{cases} -\sin(\varphi)\exp(i\psi) e_l e_q^T, & r < s \\ \sin(\varphi)\exp(-i\psi) e_l e_q^T, & r > s \end{cases}, \\ U_{sr}(k,p) &= -(U_{rs}(k,p))^H\ . \end{aligned} \tag{5}$$

Let for $r = s$

$$U_{rr}(k,p) = \begin{cases} T = T(l;q;\varphi;\psi), & 1 \le p \le b(b-1)/2 \\ T & p > (b(b-1)/2 \end{cases} \tag{6}$$

where $\varphi = \varphi(r;s;l;q)$, $\psi = \psi(r;s;l;q)$, e_l and e_q are corresponding vector colums of the unit $b \times b$ matrix I. The matrix $P_{l,q}$ is a permutation matrix which rearranges l and q rows and colums. The matrix $T(l;q;\varphi;\psi;)$, $i,j = 1,\ldots,b$ is chosen so that $t_{ij} = \delta_{ij}$ for $(i,j) \notin \{(l,l),(q,q),(l,q),(q,l)\}$ and $t_{ll} = t_{qq} = \cos(\varphi)$, $t_{lq} = -\bar{t}_{ql} = -\sin(\varphi)\exp(i\psi)$.

Next we are going to show how to determine pairs (r,s) and (l,q).

Let n be an even number and $m = n/2$.

Now we choose the indices (r, s) of the blocks for $k = 0, 1, \ldots, 2m$ by using the following formulas:

$$
(7)\quad
\begin{array}{ll}
\text{a)} & \text{if } k = 0, \text{ then } r = s = 1, 2, \ldots, n/2. \\
\text{b)} & \text{for } k = 1, 2, \ldots, m-1 \\
& \quad s = m-k+1,\ m-k+2, \ldots, n-k \\
& \quad r = 2m-2k+1-s, \qquad m-k+1 \le s \le 2m-2k \\
& \quad r = 4m-2k-s, \qquad 2m-2k < s \le 2m-k-1 \\
& \quad r = n, \qquad 2m-k = s
\end{array}
$$

$$
\begin{array}{ll}
\text{c)} & \text{for } k = m, \ldots, 2m-1 \\
& \quad s = 4m-n-k,\ 4m-n-k+1,\ \ldots,\ 3 \qquad m-k-1 \\
& \quad r = n, \qquad s = 2m-k \\
& \quad r = 4m-2k-s, \qquad 2m-k+1 \le s \le 4m-2k-1 \\
& \quad r = 6m-2k-s, \qquad 4m-2k-1 < s \\
\text{d)} & \text{if } k = 2m, \text{ then } r = s = n/2+1, \ldots, n.
\end{array}
$$

Let n be an odd number and $m = (n+1)/2$. Then we choose (r, s) for $k = 1, 2, \ldots, 2m-1$ as follows:

$$
(8)\quad
\begin{array}{ll}
\text{a)} & \text{let } k = 1, 2, \ldots, m-1 \\
& \quad s = m-k+1,\ m-k+2, \ldots, n-k, \qquad n-k+1 \\
& \quad r = 2m-2k+1-s, \qquad m-k+1 \le s \le 2m-2k \\
& \quad r = 4m-2k-s, \qquad 2m-2k < s \le 2m-k-1 \\
& \quad r = 2m-k, \qquad s = 2m-k \\
\text{b)} & \text{let } k = m, \ldots, 2m-1 \\
& \quad s = 4m-n-k-1,\ 4m-n-k,\ \ldots,\ 3 \qquad m-k-1 \\
& \quad r = 2m-k \qquad s = 2m-k \\
& \quad r = 4m-2k-s, \qquad 2m-k+1 \le s \le 4m-2k-1 \\
& \quad r = 6m-2k-s, \qquad 4m-2k-1 < s
\end{array}
$$

Having found pairs (r, s) through the above formulas we have to choose the indices l, q of the elements in the blocks (r, s):

a) if $r \neq s$, then

$$(l, q) = \left[(1,1), (1,2), \ldots, (1,b), (2,1), (2,2), \ldots, (b,1), \ldots, (b,b)\right].$$

b) if $r = s$, then

$$(l, q) = \left[(1,2), \ldots, (1,b), (2,3), \ldots, (2,b), \ldots, (b-1,b)\right].$$

2. Examples. 1. If $n = 6$ then $m = 3$. If $k = 3$, then the positions (r, s) of the non-zero blocks obtained from (7) are $(r, s) = [(1,5),(2,4),(6,3)]$. The matrix $U_3 = \prod_{p=1}^{b*b} U_{3p}$, U_{3p} for each p is of the type

$$U_{3p} = \begin{pmatrix} * & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & * & \cdot & \cdot \\ \cdot & \cdot & * & \cdot & \cdot & * & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & * & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & * \\ \cdot & \cdot & * & \cdot & \cdot & * & \cdot & \cdot & \cdot & \cdot & \cdot \\ * & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & * & \cdot & \cdot \\ \cdot & \cdot & \cdot & * & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & * \end{pmatrix},$$

where the non-zero blocks of U_{3p} obtained from (5) are denoted by "$*$".

2. If $n = 6$ then $m = 3$. If $k = 6$, then the positions (r, s) of the non-zero blocks obtained from (7) are $[(4,4),(5,5),(6,6)]$. The matrix $U_{6p} = \prod_{p=1}^{\alpha_6} U_{6p}$, $\alpha_6 = b(b-1)/2$, U_{6p} for each p is of the type

$$U_{6p} = \mathrm{diag}\,[I, I, I, T_4, T_5, T_6]$$

where $T_i = T(l; q; \varphi_i; \psi_i)$, $i = 4,5,6$ are blocks of type (6).

3. If $n = 5$ then $m = 3$. If $k = 5$, then the positions (r, s) of the non-zero blocks obtained from (8) are $(r, s) = [(1,1),(5,2),(4,3)]$. The matrix $U_s = \prod_{p=1}^{b*b} U_{5p}$, U_{5p} for each p is of the type

$$U_{5p} = \begin{pmatrix} * & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & * & \cdot & \cdot & \cdot & \cdot & * \\ \cdot & \cdot & * & \cdot & * & \cdot & \cdot \\ \cdot & \cdot & * & \cdot & * & \cdot & \cdot \\ \cdot & * & \cdot & \cdot & \cdot & \cdot & * \end{pmatrix},$$

where the non-zero blocks of U_{5p} obttained from (6) are denoted by "$*$".

Pairs (r, s) and (l, q) for the matrix A are determined as in Jacobi's mathod for scalar matrices with, cyclic choice of indices. The convergence for Jacobi's cyclic method is proved by Henrici [2]. In this case matrix A is reduced to a diagonal matrix. A diagonal form of A is obtained by using some criteria for convergence given in [4] in β sweep. The approximate eigenvalues of A are situated on the main diagonal of $A_3 = W^H AW$. The columns of $W = \prod_{s=0}^{\beta-1} U^{(s)}$ are the corresponding eigenvectors.

The parallel method may be implemented when working on computer ILLIAC IV.

3. Numerical Results. Numerical experiments are accomplished with real symmetric matrices, whose elements are random numbers in the interval $(0, 1]$ for $nb = 16, 32, 48, 64, 72$. Ten experiments have been made for each nb by three programs. The first program is program NBCJ for the above algorithm. The second program is that of

Jacobi for Sameh's algorithm used on sequential computer. The third involves program TRED2/TQL2 [5]. All the results obtained have been compared.

The conditions of the experiments are similar to those described in [1]. The average time for computing the eigenvalues thought TRED2/TQL2 is $5, 30, 99, 230, 320$ seconds for $nb = 16, 32, 48, 64, 72$ respectively. The avarage time for computing the eigenvalues by Jacobi's program is $9, 72, 246, 600, 865$ seconds for $nb = 16, 32, 48, 64, 72$ respectively. Table 1 shows the average number of scalar rotations with Jackobi's and NBCJ mehtods. Figure 1 shows the average time of the execution of the three programs used (TRED2/TQL2, Jacoby, NBCJ). Figure 2 shows the ratio between the average number of rotations (NBCJ) and the average number of rotations (Jacobi) (see Table 1). Figure 2 shows the ratio between the average number of rotations BCJ and the averadge number of rotations (Jacobi) (see Table 2 [1]).

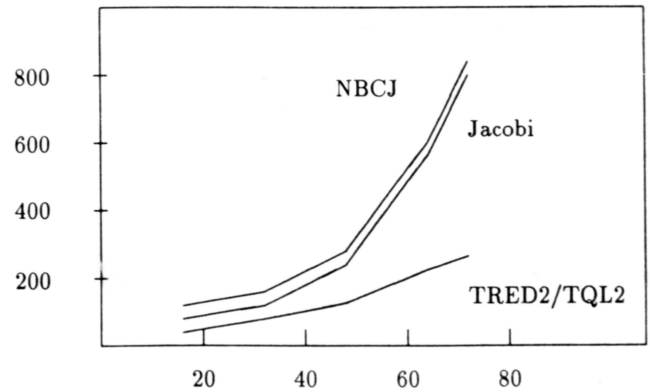

Figure 1. Average solution time for $nb = 16, 32, 48, 64, 72$.

The results given in the figures and the Table 1 show that the algorithm offered for block Hermitian matrices is more effective than BCJ mehtod [1]. The time and the number of the scalar rotations with BCJ depend on the size of block b, while they do not depend on that size NBCJ.

nb	b	Jacobi AVG	NBCJ AVG
16	4	624	629
32	2	2976	2981
48	4	7162	7129
64	4	13530	13667
72	8	17444	17668

Table 1. Average number of scalar rotations (Jacobi and NBCJ) 10 trials.

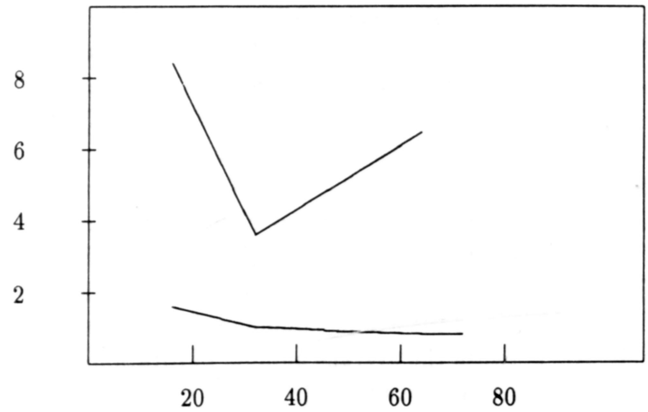

Figure 2. (Avg. rot. NBCJ)/(Avg. rot. Jacobi) from Table 1
(Avg. rot. BCJ)/(Avg. rot. Jacobi) from Table 2 [1]

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