On the Complex HZ Method for PGEP

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Abstract. The paper considers a Jacobi-type method for solving the generalized eigenvalue problem $Ax = \lambda Bx$, where A and B are complex Hermitian matrices and B is positive definite. The method is a proper generalization of the standard Jacobi method for Hermitian matrices since it reduces to it when B is diagonal. Originally, it is a two-sided method, but it can be implemented as one-sided method and then it solves the generalized singular value problem. To further enhance its efficiency on contemporary CPU and GPU architectures, it can be implemented as a block Jacobi-type method. The one-sided block method has proved to be very efficient and compares favorably to the LAPACK DTGSJA algorithm. There are several open problems related to the original method and more to its one-sided and block versions. The problems refer to the global and asymptotic convergence, high relative accuracy and speed. The aim of this short communication is to briefly describe the element-wise method and to report how well it is understood.

INTRODUCTION

The method is devised to solve the positive definite generalized eigenvalue problem (PGEP)

$$Ax = \lambda Bx\,, \quad x \neq 0\,, \tag{1}$$

where A and B are Hermitian matrices of order n and B is positive definite. The idea of the element-wise method has been briefly outlined by Zimmermannn [1] and the algorithm has been derived and analyzed by Hari [2]. In particular, the asymptotic quadratic convergence of the method under the general cyclic and the serial pivot strategies has been proved in [2]. The method is related to the Falk-Langemeyer (FL) method [3], since they both are diagonalization methods for the generalized eigenvalue problem. Like the FL method, the HZ method diagonalizes the pivot submatrices at each step. But instead of simplifying the transformation matrices (by requiring ones along the diagonal) it simplifies the iterations $B^{(k)}$ (also by requiring ones along the diagonal). So, the preliminary step for the HZ method reduces the diagonal elements of B to ones by the diagonal congruence transformation

$$A \mapsto A^{(0)} = DAD, \quad B \mapsto B^{(0)} = DBD, \quad D = \operatorname{diag}\left(b_{11}^{-1/2}, b_{22}^{-1/2}, \ldots, b_{nn}^{-1/2}\right). \tag{2}$$

Then $(A^{(0)}, B^{(0)})$ is taken as the initial pair for the algorithm.

Each of these two approaches has its advantages and shortcomings. The advantage of the FL method is that it is defined for a more general initial matrix pair, the so called definite pair. A pair of Hermitian matrices (A, B) is definite provided that $\alpha A + \beta B$ is positive definite for some real α and β. Also, each step of the method requires somewhat less flops because the diagonal elements of the transformation matrix are ones. Its asymptotic quadratic convergence and stability have been proved in [4] and [5], respectively. The shortcoming of the FL method lies in the fact that norms of the iteration matrices $A^{(k)}$ and $B^{(k)}$ increase. So, periodically one has to check the norms of $A^{(k)}$ and $B^{(k)}$, and decide whether to apply an appropriate congruence transformation to "normalize" them. This slows down the computation, especially on distributed memory parallel machines, because each check for renormalization costs. And there is no simple rule when to make a check, since it depends on the characteristics of the matrices. Also, the Fl method for complex matrices has not yet been published.

On the contrary, the HZ method has no problem with renormalizations. It is a proper generalization of the standard Jacobi method. Its real and complex algorithms have been derived in [2], where also the asymptotic quadratic

convergence has been proved for the case of simple eigenvalues. Since its real algorithm is specially related to the FL method [2], the HZ method should have the same stability property. The shortcoming of the method lies in a little more expensive transformations. Actually, this is no drawback since numerical tests on large matrices, on parallel machines, have confirmed the advantage of the HZ approach. In [6], the real method has been implemented as one-sided block method for the generalized singular value problem. Then it is almost perfectly parallelizable, so parallel shared memory versions of the algorithm are highly scalable, and their speedup almost solely depends on the number of cores used.

Since the original element-wise method is relatively unknown, this short report is devoted to shed some light on it. The element-wise method has its own merit, although it nicely fits for the role of the kernel algorithm for the block method. Here we briefly present the algorithms of the complex and real method. They both are more complicated than those for the standard complex and real Jacobi algorithms. In the final stage of the process some new phenomena can appear, which are not met by the standard Jacobi method, and which may have impact on accuracy and speed of the method. Our aim is to shed more light to those problems.

The paper is divided into three sections. In the next one, we briefly present the algorithms. In the third one, we briefly report on those new phenomena, and how they can influence the performance of the method.

Description of the Method

Let A and B be complex Hermitian matrices of order n and let B be positive definite. The initial step of the method is described by the relation (2). The HZ method is iterative process of the form

$$A^{(k+1)} = F_k^* A^{(k)} F_k, \qquad B^{(k+1)} = F_k^* B^{(k)} F_k, \qquad k \geq 0, \tag{3}$$

where $A^{(0)}$ and $B^{(0)}$ are defined by (2). In the relation (3) each transformation matrix F_k is an elementary plane matrix. It is a nonsingular matrix which differs from the identity matrix I_n in two diagonal elements $f^{(k)}_{i(k)i(k)}$, $f^{(k)}_{j(k)j(k)}$ and the two corresponding off-diagonal elements $f^{(k)}_{i(k)j(k)}$, $f^{(k)}_{j(k)i(k)}$, where $1 \leq i(k) < j(k) \leq n$. The subscripts $i = i(k)$, $j = j(k)$ are called *pivot indices*, (i, j) is *pivot pair* and

$$\hat{F}_k = \begin{bmatrix} f^{(k)}_{ii} & f^{(k)}_{ij} \\ f^{(k)}_{ji} & f^{(k)}_{jj} \end{bmatrix}, \quad k \geq 0, \tag{4}$$

is *pivot submatrix* of F_k. If $\hat{F}_k$ is as in (4), we shall denote it by $\hat{F}_k = (f^{(k)}_{ij})$. The transition $(A^{(k)}, B^{(k)}) \mapsto (A^{(k+1)}, B^{(k+1)})$ is called the kth *step* of the method. The way of selecting pivot pairs $(i(k), j(k))$ is called *pivot strategy*. The most common (pivot) strategies are the column- and row-cyclic ones, which consist of repeating $N = n(n-1)/2$ steps which make one *cycle* of the method. For the column-cyclic strategy the cycle is defined by the sequence of pivot pairs $(1,2)$, $(1,3)$, $(2,3)$, $(1,4)$, $(2,4)$, $(3,4)$, $\ldots$, $(1,n)$, $(2,n)$, $\ldots$, $(n-1,n)$, while for the row-cyclic one by $(1,2)$, $(1,3)$, $\ldots$, $(1,n)$, $(2,3)$, $(2,4)$, $\ldots$, $(2,n)$, $(3,4)$, $\ldots$, $(n-1,n)$. The common name for these two pivot strategies is *serial* (pivot) strategies. The transition $(A^{((t-1)N+1)}, B^{((t-1)N+1)}) \mapsto (A^{(tN)}, B^{(tN)})$ is called the tth *cycle* or *sweep*.

The algorithm for computing the elements of $\hat{F}_k$ is derived in [2]. It is based on the following theorem, which is a generalization to complex matrices, of the Gose's result [7].

Theorem 1 ([8]) *Let $\hat{B} = (b_{ij})$ and $\hat{B}' = diag(b'_{ii}, b'_{jj})$ be positive definite Hermitian matrices of order two. Then there exist a nonsingular matrix $\hat{F}$ of order two, such that $\hat{B}' = \hat{F}^* \hat{B} \hat{F}$. Each $\hat{F}$ satisfying that property has the form*

$$\hat{F} = \frac{1}{\cos\gamma} \begin{bmatrix} \frac{1}{\sqrt{b_{ii}}} & \\ & \frac{1}{\sqrt{b_{jj}}} \end{bmatrix} \begin{bmatrix} \cos\phi & e^{\imath\alpha}\sin\phi \\ -e^{-\imath\beta}\sin\psi & \cos\psi \end{bmatrix} \begin{bmatrix} e^{\imath\omega_i}\sqrt{b_{ii}}' & \\ & e^{\imath\omega_j}\sqrt{b_{jj}}' \end{bmatrix}, \tag{5}$$

where ω_i, ω_j are real, $\phi, \psi, \gamma \in [0, \frac{\pi}{2}]$, $\sin\gamma = \frac{|b_{ij}|}{\sqrt{b_{ii}b_{jj}}}$, and $|\cos\phi\cos\psi + e^{\imath(\alpha-\beta)}\sin\phi\sin\psi| = \cos\gamma$ holds.

To simplify $\hat{F}$, we can require that $\omega_i = \omega_j = 0$, i.e. that the diagonal elements of $\hat{F}$ are real and nonnegative.

Let $A^{(k)} = (a^{(k)}_{lr})$, $B^{(k)} = (b^{(k)}_{lr})$, $k \geq 0$. At step k the matrix F_k is sought to satisfy the following conditions

$$a^{(k+1)}_{ij} = 0, \quad b^{(k+1)}_{ij} = 0, \qquad b^{(k+1)}_{ii} = 1, \quad b^{(k+1)}_{jj} = 1, \qquad f^{(k)}_{ii} \geq 0, \quad f^{(k)}_{jj} \geq 0, \tag{6}$$

where $i = i(k)$, $j = j(k)$ for every $k \geq 0$. Since the diagonal elements of each $B^{(k)}$ are ones, the matrix $\hat{F}_k$ is sought in the form

$$\hat{F}_k = \frac{1}{\sqrt{1 - |b_{ij}^{(k)}|^2}} \begin{bmatrix} \cos\phi_k & e^{\imath\alpha_k}\sin\phi_k \\ -e^{-\imath\beta_k}\sin\psi_k & \cos\psi_k \end{bmatrix}. \tag{7}$$

In [2], $\hat{F}_k$ has been looked for in the form $\hat{F}_k = \hat{R}_1^{(k)}\hat{D}^{(k)}\hat{R}_2^{(k)}\hat{\Phi}^{(k)}$. Here $\hat{R}_1^{(k)}$, $\hat{R}_2^{(k)}$ are complex rotations and $\hat{D}^{(k)}$, $\hat{\Phi}^{(k)}$ are diagonal matrices, $\hat{\Phi}^{(k)}$ being also unitary. The rotation $\hat{R}_1^{(k)}$ is used as Jacobi rotation to diagonalize the pivot submatrix $\hat{B}^{(k)}$. Since the transformed $\hat{B}^{(k)}$ by $\hat{R}_1^{(k)}$, does not necessarily have ones on the diagonal, the transformation with $\hat{D}^{(k)}$ is used to make them 1 again. Now, $\hat{B}^{(k)}$ has become identity matrix of order 2 and $\hat{R}_2^{(k)}$ is used to diagonalize the (already) transformed $\hat{A}^{(k)}$. Finally, $\hat{\Phi}^{(k)}$ is used to make the diagonal elements of $\hat{F}_k$ nonnegative. The described procedure yields the following formulas for the elements of $\hat{F}_k$ (see [2]) which we present in the form suitable for programming.

Set

$$b_k = |b_{ij}^{(k)}|, \quad t_k = \sqrt{1 - b_k^2}, \quad e_k = a_{jj}^{(k)} - a_{ii}^{(k)}, \quad \epsilon_k = \begin{cases} 1, & e_k \geq 0 \\ -1, & e_k < 0 \end{cases}. \tag{8}$$

Compute u_k, v_k, $\cos\gamma_k$, $\sin\gamma_k$, $\cos 2\theta_k$, $\sin 2\theta_k$, $\cos\phi_k$, $\sin\psi_k$, $e^{\imath\alpha_k}\sin\phi_k$, $e^{-\imath\beta_k}\sin\psi_k$, where

$$\left.\begin{aligned} u_k + \imath\, v_k &= e^{-\imath\arg(b_{ij}^{(k)})}\, a_{ij}^{(k)}, \qquad \tan\gamma_k = 2\epsilon_k \tfrac{v_k}{e_k}, \quad -\tfrac{\pi}{2} < \gamma_k \leq \tfrac{\pi}{2} \\ \tan 2\theta_k &= \epsilon_k \tfrac{2u_k - (a_{ii}^{(k)} + a_{jj}^{(k)})b_k}{t_k\sqrt{e_k^2 + 4v_k^2}}, \quad -\tfrac{\pi}{4} < \theta_k \leq \tfrac{\pi}{4} \\ 2\cos^2\phi_k &= 1 + b_k\sin 2\theta_k + t_k\cos 2\theta_k\cos\gamma_k, \qquad 0 \leq \phi_k \leq \tfrac{\pi}{2} \\ 2\cos^2\psi_k &= 1 - b_k\sin 2\theta_k + t_k\cos 2\theta_k\cos\gamma_k, \qquad 0 \leq \psi_k \leq \tfrac{\pi}{2} \\ e^{\imath\alpha_k}\sin\phi_k &= \tfrac{e^{\imath\arg(b_{ij}^{(k)})}}{2\cos\psi_k}\left[\sin 2\theta_k - b_k - \imath t_k\cos 2\theta_k\sin\gamma_k\right] \\ e^{-\imath\beta_k}\sin\psi_k &= \tfrac{e^{-\imath\arg(b_{ij}^{(k)})}}{2\cos\phi_k}\left[\sin 2\theta_k + b_k + \imath t_k\cos 2\theta_k\sin\gamma_k\right]. \end{aligned}\right\} \tag{9}$$

Execute the transformation (3), with F_k determined by $\hat{F}_k$ whose elements are given by the relations (7)—(9).

If $b_{ij}^{(k)} = 0$, then in the above formulas $\arg(b_{ij}^{(k)})$ is replaced by $\arg(a_{ij}^{(k)})$. Then $\hat{F}_k$ is reduced to the (complex) Jacobi rotation for $\hat{A}^{(k)}$. If in addition $a_{ij}^{(k)} = 0$, then $u_k = v_k = \gamma_k = \theta_k = \phi_k = \psi_k = 0$, hence F_k is the identity matrix.

If A and B are real, then $A^{(k)}$, $B^{(k)}$ and F_k are real for all $k \geq 0$. In that case the algorithm simplifies. In particular, in the relation (7) we have $\alpha_k = \beta_k = 0$, the relation (8) is replaced by

$$\xi = \frac{b_{ij}^{(k)}}{\sqrt{1 + b_{ij}^{(k)}} + \sqrt{1 - b_{ij}^{(k)}}}, \qquad \eta = \frac{b_{ij}^{(k)}}{(1 + \sqrt{1 + b_{ij}^{(k)}})(1 + \sqrt{1 - b_{ij}^{(k)}})} \tag{10}$$

and the relation (9) is replaced by

$$\left.\begin{aligned} \tan 2\theta_k &= \tfrac{2a_{ij}^{(k)} - (a_{ii}^{(k)} + a_{jj}^{(k)})\, b_{ij}^{(k)}}{\sqrt{1 - (b_{ij}^{(k)})^2}(a_{jj}^{(k)} - a_{ii}^{(k)})}, \quad -\tfrac{\pi}{4} < \theta_k \leq \tfrac{\pi}{4} \\ \cos\phi_k &= \cos\theta_k + \xi_k(\sin\theta_k - \eta_k\cos\theta_k), \qquad \sin\phi_k = \sin\theta_k - \xi_k(\cos\theta_k + \eta_k\sin\theta_k) \\ \cos\psi_k &= \cos\theta_k - \xi_k(\sin\theta_k + \eta_k\cos\theta_k), \qquad \sin\psi_k = \sin\theta_k + \xi_k(\cos\theta_k - \eta_k\sin\theta_k). \end{aligned}\right\} \tag{11}$$

To measure advancement of the method, we can use the measure $S(A,B) = \left[\|A - \mathrm{diag}(A)\|_F^2 + \|B - \mathrm{diag}(B)\|_F^2\right]^{1/2}$, where $\|X\|_F = \sqrt{\mathrm{trace}(\overline{X^*X})}$ is the Frobenius norm of X. The HZ method is convergent on the pair (A,B) if the sequence of generated pairs satisfies $(A^{(k)}, B^{(k)}) \to (\Lambda, I_n)$, where Λ is diagonal and I_n is the identity. It converges globally if it converges on every (positive definite) initial pair. The cyclic method is (asymptotically) quadratically convergent if

$$S(A^{(N)}, B^{(N)}) \leq c_n S^2(A^{(0)}, B^{(0)}) \quad \text{whenever } S(A^{(0)}, B^{(0)}) \text{ is sufficiently small.}$$

Here c_n is a constant which may depend on n.

Latest Research

Lately, we have considered several theoretical problems related to the element-wise HZ method. The first one is the global convergence problem under a new large class of *generalized serial strategies* and under the class of quasi-cyclic strategies that is related to it (see [9, 10]). These classes of pivot strategies include the known weak-wavefront strategies. So far, the global convergence of the Jacobi-type processes has been considered almost exclusively for the serial strategies. Now we have much larger classes of "convergent" cyclic and "convergent" quasi-cyclic strategies. To obtain those classes, we have used a new equivalence relation on the set of pivot strategies (permutation equivalence), a new notion of inverse (or reverse) pivot strategy, and tools such as Jacobi annihilators and operators. So far, we have proved the global convergence of the real and complex HZ method under those new classes of pivot strategies. We hope to obtain the same result for the block HZ methods.

The second research which is underway is the stability of the real and complex HZ method. We would like to prove high relative accuracy of the two-sided, element-wise methods in the case when the both matrices are positive definite and well behaved. This means that $\kappa_2(D_A A D_A) \ll \kappa_2(A)$, $\kappa_2(D_B B D_B) \ll \kappa_2(B)$ holds for some diagonal D_A, D_B, and $\kappa_2(X)$ is the spectral condition of X. Once we have it proved, we can use it to prove the same for the block methods, since then their kernel algorithms will have high relative accuracy. This would be an extension of the known result for the case when B is identity. That problem is somewhat challenging because we have an intrinsic instability in the formulas when the pair (A, B) has multiple eigenvalues and the matrices $A^{(k)}$, $B^{(k)}$ are almost diagonal. If $\hat{A}^{(k)}$ lies within a diagonal block associated with a multiple eigenvalue, then we shall have severe cancelation in the numerator and denominator of the quotient which defines $\tan 2\theta_k$. This deteriorates relative accuracy of the computed $\cos\theta$ and $\sin\theta$ and thus of the elements of $\hat{F}_k$. This inaccuracy alone has bad impact on the reduction of $S(A^{(k)}, B^{(k)})$, hence the process will be prematurely stalled. That results in inaccuracy of the output data.

Even worse, all the elements of $\hat{F}_k$ will be large, which will preclude the quadratic asymptotic convergence of the method. This is our third problem we deal with. For the method it means severe convergence slowdown and premature termination of the process (too many sweeps). This results not only in inaccurate output data, but in low efficiency of the method (slower and inaccurate). To solve the second and third problem, a subtle error analysis is needed which will precisely point to when, where and how to modify the method to avoid the drawback of loss of the asymptotic quadratic convergence and high relative accuracy of the method.

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