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Jacobi-Davidson Methods for Generalized MHD-Eigenvalue Problems

A Jacobi-Davidson algorithm for computing selected eigenvalues and associated eigenvectors of the generalized eigenvalue problem $Ax = \lambda Bx$ is presented. In this paper the emphasis is put on the case where one of the matrices, say the B-matrix, is Hermitian positive definite. The method is an inner-outer iterative scheme, in which the inner iteration process consists of solving linear systems to some accuracy. The factorization of either matrix is avoided. Numerical experiments are presented for problems arising in magnetohydrodynamics (MHD).

1. Introduction and notation

In this paper we are interested in the computation of accurate approximations of exact eigenvalues $\lambda \in \mathbb{C}$ and associated eigenvectors $x \in \mathbb{C}^n$ of the generalized eigenvalue problem

$$Ax = \lambda Bx, \tag{1}$$

where A and B are $n \times n$ complex matrices. We assume that the matrices are very large, sparse and irregularly structured. In this case factorization of either matrix would be impractical for obvious reasons. In [9] the Jacobi-Davidson (JD) method for computing eigensolutions of the standard problem, $B = I$ in (1), has been presented. Here we generalize this procedure in order to solve (1) for $B \neq I$. We will emphasize on the case where B is Hermitian positive definite. A more general treatment will be presented elsewhere, see [2].

Notation. The Euclidean inner product of two vectors v and w is denoted as $(v, w) = w^*v$, the Euclidean norm of a vector v is indicated as $||v||_2 = \sqrt{(v, v)}$. For a Hermitian positive definite matrix B we define the B-inner product of two vectors v and w by $[v, w] \equiv (Bv, w)$ and the B-norm of a vector v as $||v||_B \equiv \sqrt{(Bv, v)}$. Two vectors v and w are said to be B-orthogonal if $[v, w] = 0$. If S is a subspace, then the B-orthogonal complement of S is given by $S^{\perp_B} \equiv \{v \in \mathbb{C}^n \mid [v, w] = 0 \ \ \forall w \in S\ \}$.

2. Jacobi-Davidson for standard eigenproblems

We assume for the moment that $B = I$. Suppose at a certain point in the iterative JD process we have obtained a (non-trivial) approximation u of the *true* eigenvector x associated with some *true* eigenvalue λ. We assume that $||u||_2 = 1$. The eigenvalue approximation is $\theta = u^*Au$. The residual vector is denoted as $r = Au - \theta u$. Consider the orthogonal projector $P = uu^*$ onto the subspace span$\{u\}$. Then $I - P$ is the projector onto the orthogonal complement of span$\{u\}$, which we denote by $u^\perp$. Any vector $v \in \mathbb{C}^n$ can be written as $v = v_1 + v_2$ with $v_1 \in$ span$\{u\}$ and $v_2 \in u^\perp$. Note that we have the freedom to normalize x, such that $x = u + z$ with $z \perp u$. This suggests to search for a correction vector $z \in u^\perp$. The restriction of A to $u^\perp$ is given by $A_\mathrm{P} = (I - P)A(I - P)$. Rewriting this equation, we obtain $A = A_\mathrm{P} + Auu^* + uu^*A - \theta uu^*$. Substituting this relation into eq. (1) for $B = I$ and writing $x = u + z$, we obtain, using some trivial expressions (e.g., $A_\mathrm{P}u = 0$):

$$(A_\mathrm{P} - \lambda I)z = -r + (\lambda - \theta - u^*Az)u. \tag{2}$$

Since the left-hand side of (2) is orthogonal to u and also r is orthogonal to u, the factor in front of u on the right-hand side is equal to 0, or, $\lambda = \theta + u^*Az$. Therefore (2) reduces to $(A_\mathrm{P} - \lambda I)z = -r$. The exact correction vector z cannot be computed, since we do not know the exact eigenvalue λ. However, an approximation θ is available. Therefore, we replace λ by θ and compute an approximate solution $\tilde{z}$ of

$$(A_\mathrm{P} - \theta I)z = -r, \tag{3}$$

for instance by performing a few steps of some iterative method including a suitable preconditioner. The updated eigenvector approximation is then given by $u + \tilde{z}$. This may lead to a very fast converging process, as can be seen by establishing its relation to the Rayleigh quotient iteration (RQI) method. Suppose we would solve eq. (3) exactly. The solution is then given by (see [9], or below) $z = -u + \eta(A - \theta I)^{-1}u$, with $\eta = [u^*(A - \theta I)^{-1}u]^{-1}$. The updated eigenvector approximation is then equal to $\eta(A - \theta I)^{-1}u$, which implies that the JD method becomes mathematically equivalent to RQI. This would lead to cubic convergence for Hermitian A, or quadratic convergence for non-Hermitian A, see [5,6]. In practice only a moderately accurate solution of (3) is often sufficient to retain fast convergence.

Instead of performing a single-vector iteration, i.e., replacing u by $u+\tilde{z}$, the method is accelerated by searching for the best eigenvector approximation in a subspace, as will be explained in the next section.

3. Jacobi-Davidson for generalized eigenproblems

From now on we assume $B \neq I$ and B to be Hermitian positive definite. Following the prescription of the previous section, we might search for a correction z in the orthogonal complement of span$\{u\}$. However, it is easily verified (see [2]) that this would lead to an iterative process that is not related to the RQI method. Instead we can look for a correction z in the B-orthogonal complement of span$\{u\}$, denoted as $u^{\perp_B}$.

Definition 1. A projector P onto a subspace S is said to be a B-orthogonal projector if $\mathrm{Ker}(P) = \mathrm{Ran}(P)^{\perp_B}$.

Proposition 1. *A projector P onto a subspace S is B-orthogonal if and only if it is self-adjoint with respect to the B-inner product, i.e., $[Pv, w] = [v, Pw]\ \forall\, v, w \in \mathbb{C}^n$.*

Proof. If P is B-orthogonal, then by definition we have $\mathrm{Ker}(P) = \mathrm{Ran}(I-P) = \mathrm{Ran}(P)^{\perp_B} = S^{\perp_B}$. The space $\mathbb{C}^n$ can be decomposed as the direct sum $\mathbb{C}^n = \mathrm{Ran}(P) \oplus \mathrm{Ker}(P)$. Therefore, any vector v can be written uniquely as $v = Pv + (I-P)v$ with $Pv \in S$ and $(I-P)v \perp_B S$. The self-adjointness is then easily verified, since for any two vectors v, w we have:

$$[v, Pw] \;=\; [Pv + (I-P)v, Pw] \;=\; [Pv, Pw] \;=\; [Pv, Pw + (I-P)w] \;=\; [Pv, w]\,.$$

Now we prove that the converse is true. Suppose $v \in \mathrm{Ker}(P)$. If P is self-adjoint with respect to the B-inner product, then, for any vector $w \in \mathrm{Ran}(P)$, we have $[v, w] = [v, Pw] = [Pv, w] = 0$. This implies that $v \in \mathrm{Ran}(P)^{\perp_B}$, or $\mathrm{Ker}(P) \subseteq \mathrm{Ran}(P)^{\perp_B}$. Now suppose $v \in \mathrm{Ran}(P)^{\perp_B}$. Then for any vector $w \in \mathrm{Ran}(P)$ we obtain $[v, w] = [v, Pw] = [Pv, w] = 0$. This shows that $Pv = 0$, or $v \in \mathrm{Ker}(P)$, or $\mathrm{Ker}(P) \supseteq \mathrm{Ran}(P)^{\perp_B}$. This completes the proof, since we have $\mathrm{Ker}(P) = \mathrm{Ran}(P)^{\perp_B}$, and therefore P is B-orthogonal.

We assume u to be normalized such that $||u||_B = 1$. The eigenvalue approximation $\theta = u^* Au$ and the residual vector $r = Au - \theta Bu$ is orthogonal to u. Consider the projector $P = uu^* B$. It is easy to show that P is a projector onto span$\{u\}$ and that P is self-adjoint with respect to the B-inner product. By the above proposition it follows that P is B-orthogonal. Therefore, we may write x as $x = Px + (I-P)x = \alpha u + z$ with $z \in u^{\perp_B}$. Again we can normalize x such that $\alpha = 1$. The restriction of A to $u^{\perp_B}$ is given by $A_{\mathrm{P}} = (I-P)^* A (I-P)$. Rewriting this equation for the matrix A and substituting the resulting expression for A into eq. (1), we obtain the equivalent of eq. (2):

$$(A_{\mathrm{P}} - \lambda B)z = -r + (\lambda - \theta - u^* Az)Bu. \tag{4}$$

Premultiplication on both sides of eq. (4) with u^* yields $\lambda = \theta + u^* Az$. Again we replace λ by the current approximation θ. Similarly to eq. (3), the correction vector $\tilde{z}$ is now computed as the approximate solution of

$$\{(I - Buu^*)A(I - uu^* B) - \theta B\}z = -r \quad \text{and} \quad [z, u] = 0. \tag{5}$$

Now we derive a more convenient formulation of eq. (5). First note that $(I - uu^* B)z = z$. Then (5) is equivalent to the following equation:

$$(A - \theta B)z + \varepsilon Bu = -r \quad \text{with} \quad \varepsilon = -u^* Az \quad \text{and} \quad [z, u] = 0.$$

It easy to show that the solution z of this linear system in $\mathbb{C}^n$ is identical to the vector z obtained by solving the following system in $\mathbb{C}^{n+1}$:

$$\begin{bmatrix} A - \theta B & Bu \\ u^* B & 0 \end{bmatrix} \begin{bmatrix} z \\ \varepsilon \end{bmatrix} = \begin{bmatrix} -r \\ 0 \end{bmatrix}. \tag{6}$$

Suppose K is a non-singular $n \times n$ matrix and a, b are vectors in $\mathbb{C}^n$. Then it is easily verified that in $\mathbb{C}^{n+1}$ we have

$$\begin{bmatrix} K & b \\ a^* & 0 \end{bmatrix}^{-1} = \begin{bmatrix} I & -y \\ 0^* & 1 \end{bmatrix} \begin{bmatrix} I & 0 \\ a^*/\nu & -1/\nu \end{bmatrix} \begin{bmatrix} K^{-1} & 0 \\ 0^* & 1 \end{bmatrix} \quad \text{with} \quad y = K^{-1}b \quad \text{and} \quad \nu = a^* y. \tag{7}$$

Using eq. (7) with $K = A - \theta B$ and $a = b = Bu$, we obtain the exact solution vector z of eq. (6): $z = -u + \eta(A - \theta B)^{-1}Bu$, with $\eta = [u^*B(A - \theta B)^{-1}Bu]^{-1} = -\varepsilon$. The updated eigenvector approximation $u + z$ is equal to $\eta(A - \theta B)^{-1}Bu$, which implies that the JD method for generalized eigenproblems becomes equivalent to the RQI method for the generalized case (see [5]). As for standard problems, the correction equation (6) often needs only to be solved to a moderate accuracy in order to retain reasonably fast convergence of the JD method. It should be noted that although the exact solution z of eq. (6) is B-orthogonal to u, this is of course not automatically guaranteed for an approximate solution $\tilde{z}$. However, the B-orthogonality can be nicely restored by a suitable preconditioner as shown by the following lemma.

Lemma 1. *Suppose an approximate solution of the augmented linear system (6) is computed by performing a few iteration steps of a Krylov subspace method, starting with initial guess 0. Assume the system to be left-preconditioned according to eq. (7) with $a = b = Bu$ and K some approximation of $A - \theta B$. Then the approximate solution $(\tilde{z}, \tilde{\varepsilon})^*$ of eq. (6) is such that $\tilde{z}$ is B-orthogonal to u.*

Proof. A straightforward calculation of the vectors spanning the Krylov subspace yields only vectors in $\mathbb{C}^{n+1}$ of which the first n components form a vector in $\mathbb{C}^n$ that is B-orthogonal to u. Since the initial guess is 0 the vector $(\tilde{z}, \tilde{\varepsilon})^*$ is in the Krylov subspace and therefore the approximate solution $\tilde{z}$ is B-orthogonal to u.

The method is accelerated by searching for the best eigenvector approximation in the subspace spanned by the initial guess for the eigenvector and all the correction directions. If $v_1, \ldots, v_k$ is a basis for this subspace obtained after k JD iterations and V_k denotes the $n \times k$ matrix with these basis vectors as its columns, then the eigenvector approximation $u = V_k s$ associated with the eigenvalue approximation θ is obtained by solving the $k \times k$ projected generalized eigenvalue problem:

$$V_k^* A V_k s = \theta V_k^* B V_k s \quad \text{with} \quad s \in \mathbb{C}^k. \tag{8}$$

If B is Hermitian positive definite, we are able to construct a B-orthonormal basis, i.e., $V_k^* B V_k = I_k$, and the generalized projected problem (8) reduces to a standard problem. We use modified Gram-Schmidt (see e.g. [3,6]) to B-orthogonalize vectors (denoted as *MGSB* in the algorithm below). To implement this efficiently we need to store the basis $W_k^B \equiv BV_k$. The basis $W_k^A \equiv AV_k$ is stored for the efficient computation of the projected matrix $H_k \equiv V_k^* A V_k$. The iteration process is restarted when the subspace dimension k has reached the maximum value m. The restart is carried out with the eigenvector approximation u. A possible outline of the JD procedure is given by the following algorithm.

Algorithm *Jacobi-Davidson for matrix pairs (A, B).*

0. Choose an initial vector v_1 of B-norm unity; set $V_1 = [v_1]$; set k=1;
1. Compute the last column of the matrix $W_k^A := AV_k$;
2. Compute the last column of the matrix $W_k^B := BV_k$;
3. Compute the last column and row of the projected matrix $H_k := V_k^* W_k^A$;
4. Compute a selected eigenpair (θ, s) of H_k with $||s||_2 = 1$;
5. Compute the Ritz vector $u := V_k s$ and the vectors $p := W_k^A s$ and $q := W_k^B s$;
6. Compute the residual vector $r := p - \theta q$ and $||r||_2$; `if` convergence `then` exit;
7. Compute an approximate solution $\tilde{z}$ of: $\begin{bmatrix} A - \theta B & q \\ q^* & 0 \end{bmatrix} \begin{bmatrix} z \\ \varepsilon \end{bmatrix} = \begin{bmatrix} -r \\ 0 \end{bmatrix}$;
8. `if` $k < m$ `then`
  $k := k + 1$; compute $V_k :=$*MGSB*$[V_{k-1}, \tilde{z}]$; `goto` **1**;
 `else`
  set $V_1 = [u]$, $W_1^A = [p]$, $W_1^B = [q]$, $H_1 = [\theta]$; set $k = 2$; compute $V_k :=$*MGSB*$[V_{k-1}, \tilde{z}]$; `goto` **1**;
 `end if`

In step 4 of the algorithm we need to compute eigenpairs (θ, s) of the small projected problem $H_k s = \theta s$. This can be done by the QR algorithm (see e.g. [3]). The vectors s are normalized such that $||s||_2 = 1$, which implies that $||u||_B = 1$. The selected eigenvalue may for example be the one with largest (smallest) absolute value or the one closest to a fixed point σ in the complex plane. In the latter case we refer to σ as a shift.

We have tested the algorithm on a MHD generalized eigenvalue problem taken from [4]. The A-matrix is non-Hermitian and the B-matrix is Hermitian positive definite. Both matrices are block tri-diagonal. The size of the test problem is $n = 416$, the size of the blocks is 16. In MHD problems one is interested in an interior part of the spectrum, known as the Alfvén branch. The test problem we examine here has been studied in detail with an Arnoldi method in [4] and with a Lanczos procedure in [1]. We use the algorithm given above in order to obtain an approximation for the eigenvalue closest to the shift $\sigma = -0.35 + 0.60i$. The iteration process is stopped if the residual norm of the eigenpair approximation is below 10^{-8}. The correction equation in step 7 of the algorithm is solved approximately by performing a fixed number of GMRES [8] iteration steps, starting with initial guess 0. In three different runs of the algorithm the systems are solved to some accuracy with 5, 10 and 20 GMRES steps. For the three runs we employ the same preconditioning according to eq. (7): we use $a = b = Bu$ and for K an incomplete LU factorization of $A - \sigma B$. Note that the preconditioner is computed only once and that it gets more effective during the JD process, once the eigenvalue approximation moves towards the shift. We compute an ILUT(l, τ) factorization [7]. This is based on a dual dropping strategy: τ denotes a relative drop tolerance [7], while l denotes the maximum number of elements kept in a row of the L- and U-factors (in addition to the diagonal element which is always kept). In the present example we set $l = 25$ and $\tau = 10^{-4}$. In all experiments the starting vector for the JD process is chosen as $v_1 = \alpha(1, \ldots, 1)^t$ with α such that $||v_1||_B = 1$. Finally we remark that the JD algorithm was not restarted in the experiments presented here.

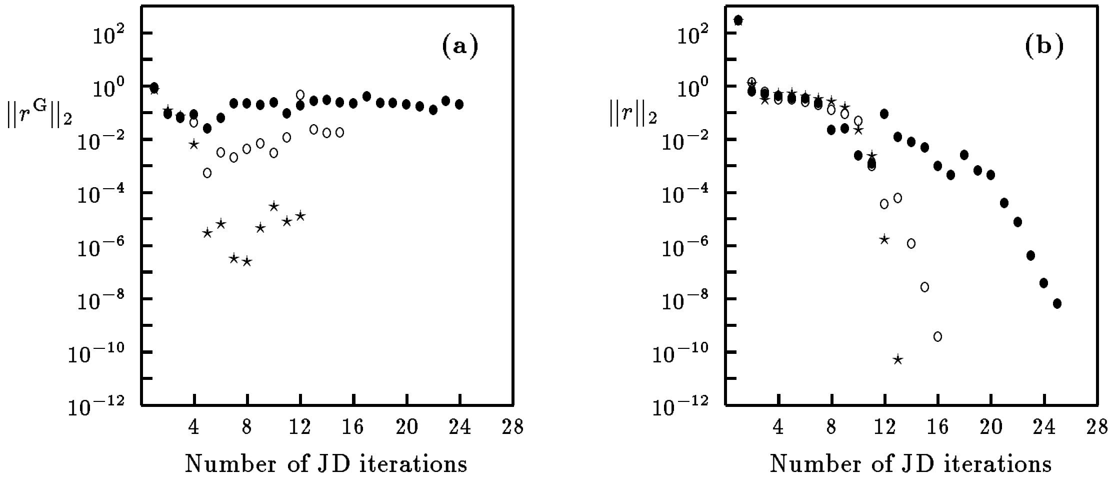

Figure 1: **(a)** Accuracy obtained for the approximate solutions of the linear systems: the reduction in the residual norm $||r^G||_2$ is shown for solving the systems with 5 ($\bullet$), 10 ($\circ$) and 20 ($\star$) GMRES steps; **(b)** convergence history for the eigenpair approximation (same notation as for **(a)**).

Figure 1 shows the results of our experiments: (a) displays the accuracy for the inner iteration process, while (b) shows the convergence history for the eigenvalue approximation. We observe that the eigenvalue is converged in fewer iterations if we increase the number of GMRES steps for the inner iteration process. For the run with GMRES(20) (denoted by $\star$ in the figure) we see that the systems are solved very well in the final iterations resulting in an (almost) asymptotically quadratic speed of convergence for the eigenvalue approximation, as was expected. However, in terms of CPU time this is not the fastest run. On a Silicon Graphics workstation we obtain: 10.8 s for GMRES(5), 10.0 s for GMRES(10) and 13.3 s for GMRES(20).

4. References

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