Subspace Iteration for Eigenproblems

Henk van der Vorst *

Abstract

We discuss a novel approach for the computation of a number of eigenvalues and eigenvectors of the standard eigenproblem $Ax = \lambda x$. Our method is based on a combination of the Jacobi-Davidson method and the QR-method. For that reason we refer to the method as JDQR. The effectiveness of the method is illustrated by a numerical example.

1 Introduction

The computation of eigenvalues and eigenvectors for the standard eigenproblem was considered a solved problem 15 years ago, as far as matrices of modest order were concerned. The situation for large matrices, say of order $n = 2,000$ or more, was less satisfactory, since these matrices can not be treated by the standard direct approaches: reduction to special form, plus QR-iteration on this special form. This requires $\mathcal{O}(n^3)$ arithmetic operations, and apart from storage considerations, it is clear that this puts limits on n. For very large sparse symmetric matrices, the iteration method of Lanczos [9] was more or less accepted around 1980, due to pioneering work of Paige [10]. Various effects in the convergence of eigenvalue approximations in the Lanczos process have been analysed in great detail in [16]. Similar methods for unsymmetric matrices were available, but their behavior is still less well understood: Arnoldi's method [1], the two-sided Lanczos method [8], and Davidson's method [4].

In the past five years we have seen great progress in the further development of these three methods. The two-sided Lanczos process was further stabilized by including a so-called look-ahead technique [11], but the method is still not very popular because of the non-orthogonal transformations and projections involved. Arnoldi's method was not so popular because of the increasing computational complexity per iteration step, but Sorensen [15] has solved this problem elegantly with an implicit restart technique by which the dimensions of the searchspaces can be kept modest. The method of Davidson was the inspiration for a new technique, which comes down to the combination of a key element in Davidson's algorithm with a very old, but not very well-known, technique of Jacobi [7], which was published 150 years ago. The novel technique was given the name Jacobi-Davidson and published in [14].

Before we give a short overview of the methods of Lanczos, Arnoldi, Davidson, and Jacobi-Davidson, we will first discuss a motivating example of very large sparse unsymmetric eigenvalue problems.

Then we will discuss briefly the novel iteration technique, based on the Jacobi-Davidson method, and we will give an example of its use.

2 An example of very large eigenproblems

Although large eigenproblems arise in many scientific problems, we have been particularly motivated by the NWO-sponsored project on MHD-problems[1]. In this project we study the dynamics

*Mathematical Institute, University of Utrecht, Budapestlaan 6, Utrecht, the Netherlands
e-mail: `vorst@math.ruu.nl`

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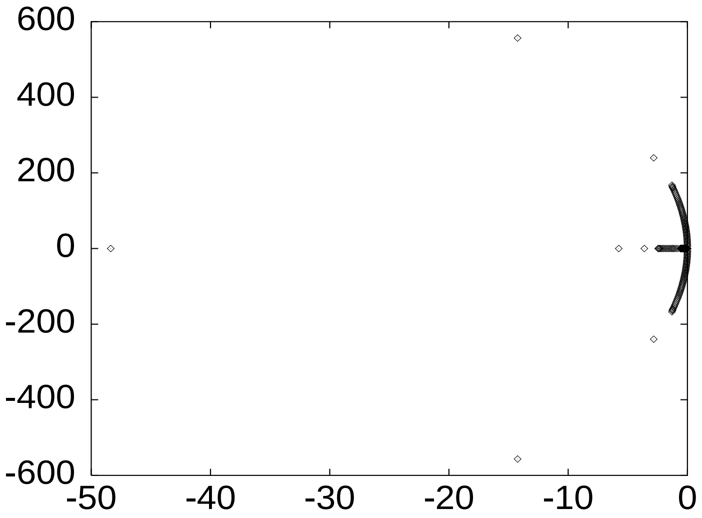

Figure 1: Eigenvalues for MHD problem

of plasmas in a magnetic field with computational models. The results are applied for further understanding of the stability of Tokomak fusion reactors and of coronal loops, as well as of solar flares.

The interaction of plasma and a magnetic field is governed by essentially the flow equations for fluids combined with the Maxwell equations, and this system has the form

$$
\begin{aligned}
\frac{\partial \rho}{\partial t} &= -\nabla \cdot (\rho \mathbf{V}) \\
\rho \frac{\partial \mathbf{V}}{\partial t} &= -\rho(\mathbf{V} \cdot \nabla)\mathbf{V} - \nabla p \\
&\quad +(\nabla \times \mathbf{B}) \times \mathbf{B} \\
\frac{\partial p}{\partial t} &= -(\mathbf{V} \cdot \nabla) p - \gamma p \nabla \cdot \mathbf{V} + \\
&\quad (\gamma - 1)\eta(\nabla \times \mathbf{B})^2 \\
\frac{\partial \mathbf{B}}{\partial t} &= \nabla \times (\mathbf{V} \times \mathbf{B}) - \nabla \times (\eta \nabla \times \mathbf{B}) \\
\text{with} \quad & \nabla \cdot \mathbf{B} = 0.
\end{aligned}
$$

The last equation is considered as an initial condition on **B**. One of the approaches, taken in our project, is to consider small perturbations of the unknowns with respect to some known equilibrium, and this leads to a linear system for the first order perturbations. The solution for this linearized system is assumed to be of the form $e^{\lambda t}$, and this leads to a large linear generalized eigenproblem.

Due to the kind of discretization we use, partly finite differences, and partly Fourier series, this leads to block tridiagonal matrices, with typically $100 - 2,000$ blocks, of size $80 - 320$ each. This amounts to matrices of orders in the range $8,000 - 640,000$.

The matrices have eigenvalues that can be grouped in very large ones (associated with 'Sound waves'), very small ones, and intermediate ones (associated with 'Alfvén' waves), and we are interested in the Alfvén spectrum. In Figure 1 we see the entire spectrum, the middle part of Figure 2 shows the 'Alfvén' spectrum (note the different scales).

The order and the structure of these matrices makes standard direct methods unpractical, and

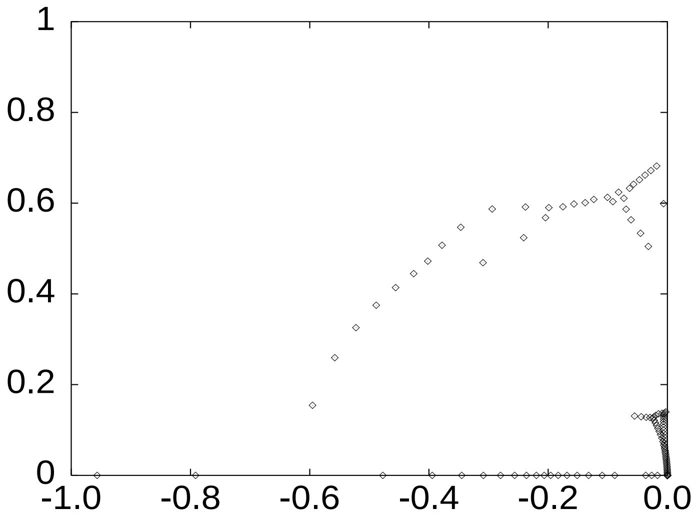

Figure 2: Alfvén part of spectrum

therefore we consider iterative methods. Similar problems have been solved up to orders of a few tens of thousands with the methods of Lanczos (with a code of Cullum et al [3]) and by Shift and Invert Implicitly Restarted Arnoldi method [15]. The applicability of these methods is limited, due to the fact that inversion of matrices is required, and this becomes too expensive for the very large problems that we are interested in. As we will see, inversion of matrices is essential for these methods in order to obtain convergence for the Alfvén spectrum.

3 Subspace Methods

For simplicity we will restrict ourselves to the standard eigenproblem $Ax = \lambda x$, with A a general matrix, and our task is to compute a few eigenvalues.
Suppose we are given a suitable low-dimensional subspace, spanned by $u_1, \ldots, u_m$. Let U_m denote the $n \times m$ matrix with u_i as its i-th column. Let us further assume that the vectors u_i form an orthonormal basis. Then the Galerkin approach is to find a vector $y \in I\!R^m$, and a θ, such that

$$AU_m y - \theta U_m y \perp \{u_1, \ldots, u_m\}$$

Since the u_i are orthonormal, this leads to an eigenproblem for a matrix of order m:

$$U_m^* A U_m y - \theta y = 0,$$

where U_m^* denotes the adjoint of U_m. In applications we have that $m \ll n$.
The solutions θ are referred to as the Ritz values (approximations for eigenvalues of A), and $U_m y$ is the corresponding Ritz vector, with respect to the subspace spanned by $u_1, \ldots, u_m$.

A very popular choice for the subspace is the so-called Krylov subspace

$$K^m(A; u_1) \equiv \{u_1, Au_1, \ldots, A^{m-1}u_1\}.$$

Note that this space is generated in the old Power iteration. After having created an orthonormal basis for the Krylov subspace: $v_1 = u_1, v_2, \ldots, v_m$, with associated matrix V_m, we obtain the projected system

$$V_m^* A V_m y - \theta y = 0.$$

If $A^* = A$ then it can be shown that $V_m^* A V_m$ is a tridiagonal matrix, and this method is known as the Lanczos method [8]. For further details see [12].

If A is unsymmetric, then the matrix $V_m^* A V_m$ becomes upper Hessenberg through Arnoldi's orthogonalization procedure [1]. For further details see [13].
The convergence of the Ritz values in these Krylov subspace methods is usually such that the exterior eigenvalues in the spectrum of A are well-approximated first. The interior eigenvalues follow much later, and in order to force an acceptable speed of convergence one has to consider the eigenproblem for $(A-\tau I)^{-1}$, in order to find interior eigenvalues close to τ. This technique is known as Shift-and-Invert, and is only practical when the shifted matrix can be inverted at relatively low costs. Note that in these Krylov subspace methods it is not necessary to invert the matrix explicitly, for the computation of $p = (A-\tau I)^{-1}q$ it is sufficient to solve p from $(A-\tau I)p = q$.

In 1975, Davidson [4] suggested an alternative for the Krylov subspace; his idea can be described as follows. Suppose that we have already a subspace of dimension m with orthonormal matrix U_m. Then we follow the Galerkin approach, and we solve the eigenproblem for the projected problem

$$U_m^* A U_m y - \theta y = 0.$$

For a pair $(U_m y, \theta)$ of interest, we compute the residual $r = AU_m y - \theta U_m y$. Originally, Davidson propsed his method for symmetric diagonally dominant matrices, so let us assume to be in that situation, and let D_A be a diagonal matrix equal to the diagonal of A. Then we compute $v = (D_A - \theta I)^{-1} r$, we orthogonalize v with respect to the columns of U_m and this gives us the new column u_{m+1}. After this step the procedure can be repeated.
The success of Davidson's method can be heuristically explained by the observation that for diagonally dominant matrices $D_A - \theta I$ is a good approximation for $A - \theta I$, so that the computation of v is an approximation for a Shift-and-Invert step. Apparantly, this is not a very satisfactory explanation, because if we take a better approximation, in particular, $v = (A-\theta I)^{-1} r$, then we see that $v = U_m y$, so that we do not expand our subspace. Lack of understanding made numerical analysts suspicious about this method, but notwithstanding this, the method was used in various circumstances with great success, also for unsymmetric systems, and with different approximations for $A - \theta I$. Another observation, namely that for $v = r$, a very poor approximation for Shift-and-Invert, we obtain formally the same results as with Arnoldi's method, so that some researchers viewed the method as a preconditioned Arnoldi method.

Recently, it was shown in [14] that the construction of an approximation for the inverse $A - \theta I$ is a wrong point of view. Instead of this it was suggested to follow an old proposal of Jacobi [7]. Jacobi made his proposal for strongly diagonally dominant matrices as a correction mechanism for the eigenvector approximation, the latter taken as the appropriate unit vector. In [14] this was for arbitrary square matrices generalized as follows. Let $(U_m y, \theta)$ be a Ritz pair with respect to U_m. Now the idea is to look for the missing complement of $u = U_m y$ in the orthogonal complement of u, denoted by $u^\perp$.
The restriction of A with respect to $u^\perp$ is given by

$$B \equiv (I - uu^*)A(I - uu^*) \quad \text{with} \quad \|u\|_2 = 1.$$

The desired correction t for u should satisfy $A(u+t) = \lambda(u+t)$, and after some trivial manipulation we find that t satisfies:

$$(B - \lambda I)t = -r,$$

for $r = Au - \theta u$.

Since λ is unknown, we approximate t by the solution $\widetilde{t}$ of $(B-\theta I)\widetilde{t} = -r$. The approximation $\widetilde{t}$ is orthogonalized with respect to U_m, which gives us an expansion vector u_{m+1}. In [14] it is proposed to solve the correction equation $(B-\theta I)\widetilde{t} = -r$ only approximately, for instance with a few steps of (preconditioned) GMRES. Numerical evidence is given that this may lead to a very effective iterative procedure, referred to as the Jacobi-Davidson method. If the correction equation is solved accurately, then we get quadratic convergence, for approximate solutions we often see linear convergence with a very small convergence factor (i.e. fast linear convergence).

4 A novel extension for the Jacobi-Davidson method

In some circumstances the Jacobi-Davidson method has apparent disadvantages with respect to Arnoldi's method. For instance, in many cases we see rapid convergence to one single eigenvalue, and what to do if we want more eigenvalues? For Arnoldi this is not a big problem, since the usually slower convergence towards a particular eigenvalue goes hand in hand with simultaneous convergence towards other eigenvalues. So after a number of steps Arnoldi produces approximations for several eigenvalues.
For Jacobi-Davidson the obvious approach would be to restart with a differently selected Ritz pair, with no guarantee that this leads to a new eigenpair. Also the detection of multiple eigenvalues is a problem, but this problem is shared with the other subspace methods.

A well-known way out of this problem is to use a technique, known as *deflation*. If an eigenvector has converged, then we continue in a subspace spanned by the remaining eigenvectors. A problem is then how to re-use information obtained in a previous Jacobi-Davidson cycle.
In [5] an algorithm is proposed by which several eigenpairs can be computed. The algorithm is based on the computation of a partial Schur form of A:

$$AQ_k = Q_k R_k,$$

where Q_k is an $n \times k$ orthonormal matrix, and R_k is a $k \times k$ upper triangular matrix, with $k \ll n$. Note that if (x, λ) is an eigenpair of R_k, then $(Q_k x, \lambda)$ is an eigenpair of A.

We now proceed in the following way in order to obtain this partial Schur form for eigenvalues close to a target value τ.
Step I: Given an orthonormal subspace basis $v_1, \ldots, v_i$, with matrix V_i, compute the projected matrix $M = V_i^* A V_i$. For the $i \times i$ matrix M we compute the complete Schur form $M = US$, with $U^*U = I$, and S upper triangular. This can be done with the standard QR algorithm [6].
Then we orden S such that the $|s_{i,i} - \tau|$ form a nondecreasing row for increasing i. The first few diagonal elements of S then represent the eigenapproximations closest to τ, and the first few of the correspondingly reordened columns of V_i represent the subspace of best eigenvector approximations. If memory is limited then this subset can be used for restart, that is the other columns are simply discarded. The remaining subspace is expanded according to the Jacobi-Davidson method.
After convergence of this procedure we have arrived at an eigenpair (q, λ) of A: $Aq = \lambda q$. The question is how to expand this partial Schur form of dimension 1. This will be shown in step II.
Step II: Suppose we have already a partial Schur form of dimension k, and we want to expand this by a convenient new column q:

$$A\,[Q_k, q] = [Q_k, q] \begin{bmatrix} R_k & s \\ & \lambda \end{bmatrix}$$

with $Q^* q = 0$.
After some standard linear algebra manipulations it follows that

$$(I - Q_k Q_k^*)(A - \lambda I)(I - Q_k Q_k^*)q = 0,$$

which expresses that the new pair (q, λ) is an eigenpair of

$$\widetilde{A} = (I - Q_k Q_k^*)A(I - Q_k Q_k^*).$$

This pair can be computed by applying the Jacobi-Davidson algorithm (with Schur form reduction, as in step I) for $\widetilde{A}$.

Some notes are appropriate:

1. Although we see that after each converged eigenpair the explicitly deflated matrix $\widetilde{A}$ leads to more expensive computations, it is shown in [5], by numerical experiments, that the entire

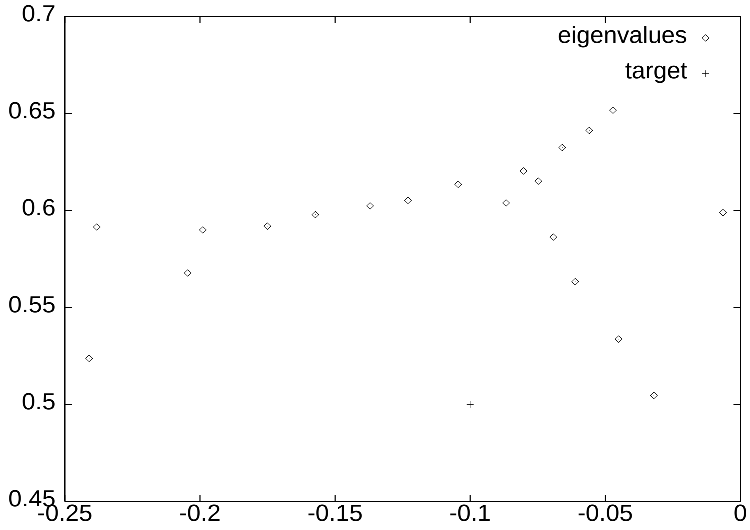

Figure 3: Computed eigenvalues

procedure leads to a very efficient computational process. An explanation for this is that after convergence of some eigenvectors, the matrix $\widetilde{A}$ will be better conditioned, so that the correction equation in the Jacobi-Davidson step is more easily solved.

2. The correction equation may be solved by a preconditioned iterative solver, and it is shown in [5] that the same preconditioner can be used with great efficiency for different eigenpairs. Hence, it pays to construct better preconditioners.

3. In [5] a similar algorithm for generalized eigenproblems $Ax = \lambda Bx$ is proposed, based on partial QZ reduction [6].

5 An example

We will now briefly describe results for the sketched approach for a generalized eigenproblem $Ax = \lambda Bx$, associated to the MHD problems discussed in Section 2. In view of the problems that we actually want to solve, our example is just a 'toy problem' of very modest dimension, $n = 416$. For more information on this particular problem, see for instance [2].

In Figure 1 we see the complete spectrum for this case; Figure 2 shows the so-called Alfvén part of the spectrum. Note the different scales from which it is obvious that the Alfvén spectrum is an interior part of the spectrum, and without Shift-and-Invert it is almost impossible to compute this part with Krylov subspace methods. The 20 eigenvalue approximations, that we have computed with the QZ-variant of our algorithm, are shown in Figure 3. The computations have been carried out in about 15 decimal digits accuracy on a SUN workstation. The target value, indicated in picture 3 by a '+', was $\tau = -.1 + .5i$. The maximum dimension of the subspaces for the Jacobi-Davidson part of the algorithm was fixed to 15. As soon as we arrived at that dimension, the subspace was shrinked, as described in **Step I** above, to 10. An eigenpair was considered to be converged as soon as the norm of the residual for the normalized eigenvector approximation was below 10^{-9}. For the preconditioner in the solution process for the correction equation, we used the exact inverse of $A - \tau B$ (for fixed τ). The correction equations were solved approximately, namely with only 1 step of GMRES. The complete converge history, norms of the residuals of eigenapproximations versus the total amount of floating point operations, is shown in Figure 4. Each time when the curve hits the 10^{-9} level, indicated by the dotted horizontal line, the algorithm has discovered a new eigenvalue. In our case that has happened 20 times, after which we have stopped the algorithm.

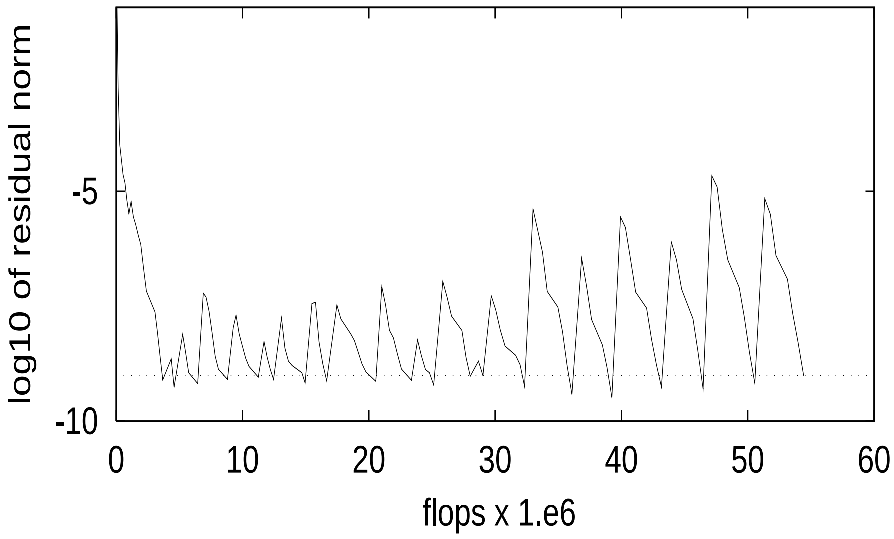

Figure 4: Convergence history

For more examples and a more thorough discussion, see [5].

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