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Davidson's algorithm with and without perturbation corrections

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Abstract. A comparison is made between Davidson's method for the real, symmetric matrix eigenproblem and a version of the Lanczos method obtained by removing the perturbation theory 'corrections' from Davidson's algorithm. It is found that the convergence of Davidson's method is superior to that of Lanczos only if the matrix is quite strongly diagonally dominant. Applications to typical matrices from nuclear structure calculations, which are not very diagonally dominant, show no essential difference between the convergence rates.

The Davidson–Lanczos method as used here is capable, unlike the usual versions of the Lanczos method, of direct application to the generalised eigenproblem $Ax = \lambda Bx$. We show how this can be implemented and give some examples that illustrate the convergence properties.

1. Introduction

Shell model calculations in nuclear physics require the computation of a small number of eigenvalues and eigenvectors, usually the extreme ones, of a real symmetric Hamiltonian matrix of high order which is only moderately sparse.

For matrices of reasonable size the problem has been completely treated in the literature (Wilkinson 1965), but for matrices of high order computational difficulties with respect to storage and rounding errors introduced in the course of computation make transformation methods unfeasible. The Lanczos method (Lanczos 1950, Paige 1972) has been found to be very efficient for the diagonalisation of such matrices and has been shown (Whitehead *et al* 1977) to be a very powerful tool in nuclear spectroscopy.

Recently, Davidson (Davidson 1975) introduced a new method and compared it to that of Lanczos. The method has been used with considerable success in molecular physics, but it is not clear that it is preferable to that of Lanczos in all cases. In particular, there are significant numerical differences between the matrices that occur in molecular and nuclear problems.

The principal aim of the present work was to investigate the claims of its originator that Davidson's method is a marked improvement over that of Lanczos. In principle Davidson's method differs from Lanczos only by the use of a device based on first-order perturbation theory (equation 2.2), the purpose of which is to accelerate convergence. The technical details of the two methods as usually presented are, however, quite different. The resulting algorithm, which we refer to as DL, is mathematically identical and numerically very similar to the standard Lanczos method. In this paper we compare

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the performance of the Davidson and DL algorithms; by switching off the Davidson perturbation correction in this way, we obtain a clear comparison of the intrinsic merits of this device.

Since the DL algorithm is no more than a variant of the Lanczos one, it might be supposed to be of no further interest. This is not the case because it turns out that this variant is applicable to the generalised eigenproblem $Ax = \lambda Bx$ in a much more straightforward way than the usual form of the Lanczos algorithm. In the following sections we describe the method together with that of Davidson and show how it can be applied to the generalised eigenproblem. Finally some numerical examples are given.

2. Description of the Davidson and DL methods

Let $U_p = (b_1, b_2, \ldots, b_p)$ be a set of $p < n$ orthonormal vectors $(n \times 1)$ and let U be the p-dimensional subspace spanned by these vectors. The methods are based on restricting the matrix A $(n \times n)$ to the subspace U and diagonalising the matrix $A_p = U_p^* A U_p$ $(p \times p)$ by some standard method (Wilkinson 1965). If U is invariant under A then the eigenvalues of A_p are equal to those of A and the corresponding eigenvectors are given by

$$x_k = U_p y_k,$$

where y_k is the kth eigenvector of A_p.

The DL algorithm for finding the kth eigenvalue $(k \leqslant p)$ and the corresponding eigenvector can be stated as follows.

(a) Form $A_p = U_p^* A U_p$ $(p \times p)$.
(b) Solve the eigenproblem $A_p y = \lambda y$. Select λ_k, y_k.
(c) Form $q_p = A U_p y_k - \lambda_k U_p y_k$.
(d) Test for convergence $(\|q_p\| < \epsilon$ or $|y_{pk}| < \epsilon)$. Stop if satisfied.
(e) Orthogonalise q_p with respect to b_i $(i = 1, \ldots, p)$. $d_{p+1} = (I - U_p U_p^*) q_p$, $b_{p+1} = d_{p+1}/\|d_{p+1}\|$.
(f) Form Ab_{p+1}, $b_i^* Ab_{p+1}$ for $i = 1, \ldots, p+1$.
(g) Repeat from step (b) with matrix A_{p+1} of order $p+1$ and $U_{p+1} = (U_p, b_{p+1})$.

Theoretically the vector q_p is orthogonal to the b_i, $i = 1, \ldots, p$, and only a normalisation is required, but rounding errors destroy the orthogonality so the orthogonalisation process is necessary. The method allows the vectors b_i, Ab_i to be kept in auxiliary store and to be transferred into the computer memory when needed.

This algorithm is mathematically equivalent (Davidson 1975) to the Lanczos method, so the results should be the same as in Lanczos apart from rounding errors. In particular as in the usual Lanczos method (Kahan and Parlett 1976) the matrix $AU_p - U_p A_p$ is null apart from its last column:

$$\begin{aligned} AU_p - U_p A_p &= (I - U_p U_p^*) A U_p = ((I - U_p U_p^*) A U_{p-1}, (I - U_p U_p^*) A b_p) \\ &= (0, (I - U_p U_p^*) A b_p), \end{aligned} \tag{2.1}$$

since by construction Ab_i $(i = 1, \ldots, p-1)$ are linear combinations of the b_i $(i = 1, \ldots, p)$. This result has been verified by numerous calculations. Thus the value of the last component of the vector y_k can be used as a stopping criterion for the process since $\|q\| = \|Ax - \lambda x\|/\|x\|$ is unsatisfactory in the case with near degenerate eigenvalues.

In Davidson's method, step (c) of the algorithm is replaced by

$$q_{ip} \leftarrow q_{ip}/(\lambda_k - a_{ii}). \tag{2.2}$$

This scheme accelerates the convergence rate considerably in the case of diagonally dominant matrices when a good approximation of the eigensolution sought is available. However, if we start with a bad subspace then the algorithm can break down (Kalamboukis 1979) since the new vector in the subspace may be almost parallel to the previous ones, causing extensive cancellation errors in the orthogonalisation process (step (d)). The vectors b_i lose their orthogonality and reorthogonalisation is necessary; even then convergence is slow. Lanczos-type results as in (2.1) cannot be applied to Davidson's method, but our numerical examples (§ 4) and other examples show that a test on the last component of the eigenvector y_k still gives a good estimate for the accuracy of the calculated eigenvectors.

3. Generalised eigenvalue problem

Consider the problem of determining a partial eigensolution of the system $Ax = \lambda Bx$ with A, B real symmetric large sparse matrices and B positive definite. The Lanczos method (Lanczos 1950) cannot be applied directly unless we factorise the matrix $B = LL^*$. In the following we propose a generalisation of the algorithms described in § 2 in which the matrices maintain their original form throughout the process. There is no need for the matrices to be declared explicitly; they can be represented in a matrix vector multiplication form in a subroutine. So we reduce the storage and the number of operations since the zeros do not appear in the multiplication. Also, it has been found in all the examples used that the vectors derived at each iteration step need not be orthogonalised as they had to be in the single eigenvalue problem.

To find the kth eigenvalue ($k \leqslant p$) one step of the algorithm can be summarised as follows: let $U_p = (b_1, \ldots, b_p)$ be p orthonormal vectors ($n \times 1$).

(a) Form $A_p = U_p^* A U_p$, $B_p = U_p^* B U_p$.
(b) Solve $A_p y = \lambda B_p y$. Select λ_k, y_k.
(c) Form $q_p = A u_p y_k - \lambda_k B U_p y_k$.
(d) Termination test ($\|q_p\| < \epsilon$). Stop if satisfied.
(e) $b_{p+1} = q_p/\|q_p\|$.
(f) Form $b_i^* A b_{p+1}$, $b_i^* B b_{p+1}$ for $i = 1, \ldots, p+1$.
(g) Continue from step (b) with matrices A_{p+1}, B_{p+1} of order $p+1$ and $U_{p+1} = (U_p, b_{p+1})$.

Theoretically the sequence of vectors b_i must terminate after n steps, but our examples show that convergence has been achieved after only a few iterations have been performed. Also the vectors b_i, Ab_i, Bb_i have to be kept in auxiliary store for later use. If any of the matrices A, B is diagonally dominant we can use Davidson's perturbation term

$$q_{ip} \leftarrow q_{ip}/(\lambda_k b_{ii} - a_{ii}) \tag{3.1}$$

instead of (c) to accelerate the convergence rate when a good approximation for the eigenvector is available. In this case orthogonalisation of the vectors b_i is necessary. However, this change (3.1) may make the algorithm unstable since the matrix B_p can lose the positive definite property in the course of computations.

4. Numerical results and discussions

In this section we shall include a few examples that give us an idea of how the methods work in practice. The eigenvalues were found using the Jacobi method for the matrix A_p and the EA11AD subroutine from the Harwell library for the generalised problem (A_p, B_p).

Example 1. We constructed a matrix (100×100) with a cluster of eigenvalues at each end of the spectrum and one single eigenvalue in between. In order to examine the convergence rate of the algorithms described we vary the dominance d of the diagonal elements $(d = \max_{i,j} \mid a_{ij}/(a_{ii} - a_{jj})|)$. The results are shown in tables 1 and 2. The values of $|y_{pk}|$ obtained from Davidson's method are compared with those obtained by applying one Lanczos step at the last iteration.

Table 1. Davidson–Lanczos algorithm.

d	Iterations	$\|q\|$	$\|y_{pk}\|$
1·0	25	$0{\cdot}1\times10^{-7}$	$0{\cdot}3\times10^{-8}$
0·1	25	$0{\cdot}5\times10^{-8}$	$0{\cdot}5\times10^{-8}$
0·01	26	$0{\cdot}4\times10^{-8}$	$0{\cdot}5\times10^{-8}$
0·001	36	$0{\cdot}3\times10^{-7}$	$0{\cdot}3\times10^{-5}$
0·0001	17	$0{\cdot}2\times10^{-7}$	$0{\cdot}5\times10^{-5}$
0·00001	8	$0{\cdot}1\times10^{-7}$	$0{\cdot}1\times10^{-7}$

Table 2. Davidson's algorithm $(q_{ip} \leftarrow q_{ip}/(\lambda_k - a_{ii}))$.

d	Iteration	$\|q\|$	$\|y_{pk}\|$ (Davidson)	$\|y_{pk}\|$ (Lanczos)
1·0	26	$0{\cdot}2\times10^{-7}$	$0{\cdot}4\times10^{-8}$	$0{\cdot}1\times10^{-8}$
0·1	24	$0{\cdot}3\times10^{-8}$	$0{\cdot}7\times10^{-8}$	$0{\cdot}1\times10^{-8}$
0·01	22	$0{\cdot}2\times10^{-8}$	$0{\cdot}2\times10^{-7}$	$0{\cdot}1\times10^{-8}$
0·001	9	$0{\cdot}1\times10^{-8}$	$0{\cdot}1\times10^{-6}$	$0{\cdot}5\times10^{-9}$
0·0001	5	$0{\cdot}3\times10^{-10}$	$0{\cdot}4\times10^{-7}$	$0{\cdot}1\times10^{-10}$
0·00001	3	$0{\cdot}1\times10^{-9}$	$0{\cdot}1\times10^{-5}$	$0{\cdot}1\times10^{-10}$

From table 2 we see that for small values of d (diagonally dominant matrix) a small value of $\|q\|$ is reached before a small value of $|y_{pk}|$. Since the accuracy of the eigenvectors depends on

$$\|q\|/\min_{i\neq j} |\lambda_i - \lambda_j|,$$

it appears that $|y_{pk}|$ gives a good indication of the accuracy of the calculated eigenvector i.e. that the factor $\min_{i\neq j} |\lambda_i - \lambda_j|$ has been effectively included by taking the step (2.2). This is emphasised by a comparison with table 1 showing the same matrix for the DL algorithm.

Example 2. A Hamiltonian matrix for ^{20}Ne i.e. two protons and two neutrons distributed in all allowed ways among the 24 single particle orbits of the nuclear *sd*-shell

(640 distinguishable states). The interaction, defined by its matrix elements in the two-body system, is the empirically determined Chung–Wildenthal interaction (Kelvin *et al* 1977) together with an empirical Coulomb interaction acting between the protons. The present method required 28 iterations to find the lowest eigenvalue with accuracy $\|q\| = 0{\cdot}5 \times 10^{-7}$ and the last component $|y_{pk}|$ equal to $0{\cdot}6 \times 10^{-8}$. The value of $|y_{pk}|$, applying one step of Lanczos method at the end, was $0{\cdot}2 \times 10^{-8}$. Davidson's method converged after 31 iterations, with $\|q\| = 0{\cdot}3 \times 10^{-7}$, and $|y_{pk}|$ for Lanczos equal to $0{\cdot}1 \times 10^{-8}$. In figure 1 we give an illustration for the convergence rate of the algorithm for the low-lying states. Note that at the last iteration six of the eigenvalues of A_p are very good approximations to those of A. In concluding, these examples and other examples tested provide us with evidence that the present method is a stable and efficient one for the eigensolution of the problem $Ax = \lambda x$ when a few of the extreme

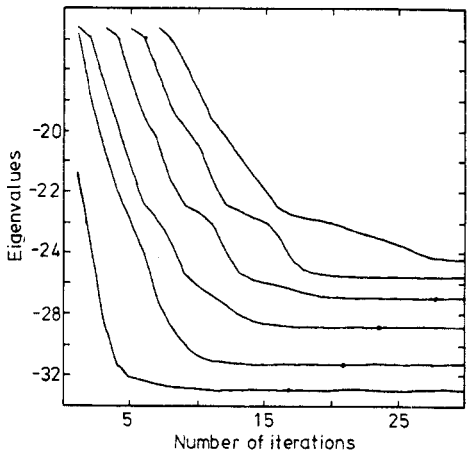

Figure 1. Convergence diagram for the lowest-lying eigenvalues of ^{20}Ne. The dots indicate the points at which eigenvalues have converged, to six significant digits.

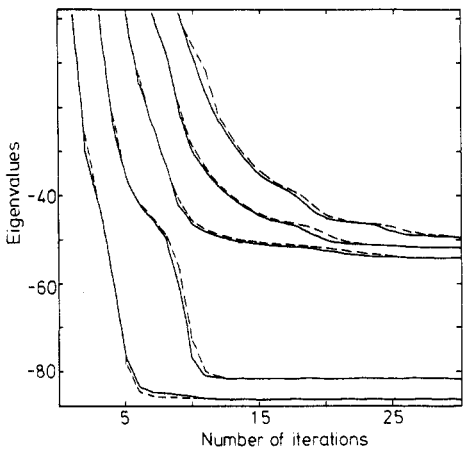

Figure 2. Convergence diagram for $Ax = \lambda Bx$ with A, B random symmetric non-diagonally dominant matrices. Continuous lines represent Davidson's generalised algorithm and broken lines the DL algorithm.

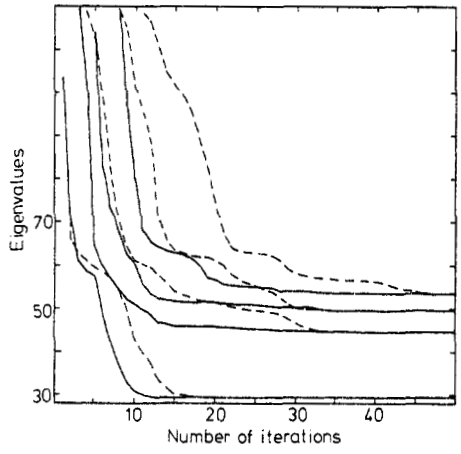

Figure 3. As for figure 2, but for diagonally dominant matrices.

eigenvalues are required, while for diagonally dominant matrices with $d < 0{\cdot}01$ Davidson's method is faster.

The examples tested for the generalised problem show the same behaviour of the algorithms as for the single case. Once again, investigation of the diagonal dominance shows that for $d < 0{\cdot}01$, for either of the matrices A, B Davidson's generalised method is faster. In figures 2 and 3 we give an illustration of the methods by presenting both cases, for diagonally and non-diagonally dominant matrices.

All of these results show clearly that no advantage is to be gained by the use of Davidson's method unless there is a considerable degree of diagonal dominance. This is not usually the case in nuclear shell-model calculations.

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