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LETTER TO THE EDITOR

Comments on the Kalamboukis tests of the Davidson algorithm

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Abstract. Conceptual errors in Kalamboukis' recent paper are pointed out. A correct outline of the Davidson algorithm is given.

In a recent paper Kalamboukis (Kalamboukis 1980) published what was purported to be a comparison between results using the Davidson algorithm (Davidson 1975) for diagonalisation of large matrices and a method he designated as Davidson–Lanczos (DL). This latter method was a version of an explicitly orthogonalised Lanczos procedure. The basic conclusion of Kalamboukis was that the Davidson algorithm was not an improvement over the Lanczos method unless the matrix was diagonally dominant. It is true that the Davidson algorithm is designed for diagonally dominant matrices (i.e. for matrices such that $|a_{ii} - a_{jj}| > |a_{ij}|$) and it would not be expected to be an improvement over the Lanczos scheme for an arbitrary matrix. In this Letter I wish to point out that the Kalamboukis version of the Davidson algorithm differs in several essentials from the version normally used and hence his numerical tests are invalid. Unfortunately Kalamboukis did not specify the matrices he used so the correct results cannot be reported here.

Kalamboukis applied his tests to the problem of finding the lowest K eigenvalues of a large matrix A of dimension n where $n \gg K$. The normal version of the Davidson algorithm when applied to this problem consists of the following steps.

Initialisation

(a) Set $p = K$.

(b) Select a set U_p of orthonormal vectors $b_1 \ldots b_K$ which approximate the first K eigenvectors of A.

(c) Construct $U_p^* A U_p$.

Iteration

(a) Solve $U_p^* A U_p Y_i = \lambda_i Y_i$, $i = 1 \ldots K$, with the eigenvalues ordered so that $\lambda_i \leqslant \lambda_{i+1}$.

(b) Test if $p+1$ exceeds the maximum size allowed for p. If so, return to the initialisation step and use the current $U_p Y_i$, $i = 1 \ldots K$, as the new $b_1 \ldots b_K$. If not, continue with step c.

(c) Select the value of k.

(d) Construct the residual error $q^{(k)}$ in the approximation $X_k = U_p Y_k$ to the kth eigenvector of A; i.e. $q_p^{(k)} = A U_p Y_k - \lambda_k U_p Y_k$.

(e) Construct the correction vector q' with elements $q'_j = q_{jp}^{(k)}/(\lambda_k - a_{jj})$.

(f) Orthogonalise q' to U_p and normalise. Insert the result into U_p and increment p. Border $U_p^* A U_p$ with a new row and column.

(g) Continue with step (a).

As Kalamboukis and Davidson both noted, if U is initialised to contain only one vector, rather than K vectors, and steps (b) and (e) are omitted, then this scheme is just an explicitly orthogonalised Lanczos method *independent of the choice of k in step* (*c*). It is this stripped down algorithm which Kalamboukis denoted as the DL algorithm. Kalamboukis mistakenly assumed, however, that merely inserting step (e) into DL would give the Davidson algorithm outlined above.

While Kalamboukis mentions k in his algorithm, it appears that he was very confused by it. As far as can be told from his paper he actually used k equal to one, but then used k in his discussions to simply label Y_i and not to refer to the k appearing in the algorithm. The basic source of his difficulty seems to have been a failure to recognise the difference in philosophy in the two methods. The Lanczos scheme attempts to find several eigenvalues from one orthogonalised Krylov sequence. The Davidson scheme uses fewer expansion vectors for each X_k but adapts the b_i separately to each value of k.

The selection of k in the Davidson algorithm may be done by any one of the following strategies. In no case is k ever left constant!

(1) Cycle k through the sequence $1 \ldots K$.

(2) Choose k to correspond to the X_j most in error as measured by the largest $|Y_{pj}|$ for $j \leq K$.

(3) Start k at one and increment k when $|Y_{pk}|$ falls below a test threshold. Method (2) will lead to the most uniform convergence of all X_i, $i = 1 \ldots K$, simultaneously.

Because the Davidson algorithm gives more rapid convergence than the Lanczos algorithm to the target vector X_k, the residuals $q_p^{(k)}$ tend to zero more rapidly and failure to change k will soon result in a vector of random numbers for the next b_{p+1}.

References

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