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Interpretation of a Linear Solver Based on Davidson's Method

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Introduction

DAVIDSON[1] originally developed an algorithm for the solution of an eigenvalue problem, which was modified and converted into a linear solver. However, no existing documentation was available on the development of this algorithm. The linear solver is an extremely efficient algorithm and is capable of solving enormous systems of equations in a very short time span. A system of 2000 equations was solved in less than 5 min, taking approximately 40 iterations.[2] This Note provides a geometric interpretation of the method and is presented as a development of the algorithm.

The Panel Method Ames Research Center program developed by NASA Ames Research Center contained a subroutine for a linear solver based on Davidson's method. The source code for this subroutine was extracted and studied, and an algorithm for the method was derived.

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Solution of Linear Systems of Equations

The following nomenclature is used: Given a system of linear equations, the coefficient matrix $\boldsymbol{A}$, the constant vector $\boldsymbol{b}$, and the solution vector $\boldsymbol{x}$ can be expressed as

$$\boldsymbol{A}\boldsymbol{x} = \boldsymbol{b} \tag{1}$$

In an iterative process, the kth iteration will be written as $\boldsymbol{x}^{(k)}$. The residual vector is

$$\boldsymbol{r}^{(k)} = \boldsymbol{b} - \boldsymbol{A}\boldsymbol{x}^{(k)} \qquad \text{for} \qquad k = 1, 2, \ldots, n \tag{2}$$

When $|\boldsymbol{r}| < \varepsilon$, convergence is assumed, where ε is the convergence criterion. Traditional solvers keep altering approximations to the solution until Eq. (2) is less than a desired tolerance ε. Another solution method involves an optimization problem. When the coefficient matrix is symmetric, the location of the absolute maximum or minimum of the associated quadratic form is equivalent to solving the linear system of equations.[3,4]

The quadratic form of Eq. (1) can be expressed as follows:

$$F(\boldsymbol{x}) = (\boldsymbol{x}, \boldsymbol{A}\boldsymbol{x})/2 - (\boldsymbol{b}, \boldsymbol{x}) \tag{3}$$

At the end of this Note, a comparison is made between the performances of the conjugate gradient (CG) method and Davidson's method using symmetric matrices. The values of the quadratic function obtained by both methods are listed along with the number of iterations taken.

Description of Davidson's Method

Davidson's method has been found to outperform the CG method. In addition, symmetry is not a prerequisite. In the CG method, asymmetric matrices must be preconditioned. The manner in which Davidson's method searches for the solution is primarily responsible for its efficiency. The CG method always conducts its search in a two-dimensional plane spanned by two orthogonal vectors. It then searches for an approximation to the solution in that plane. At the next iteration, a new search is conducted in a plane orthogonal to the previous one. This process continues until the convergence criterion has been satisfied.

Davidson's method, however, takes this idea one step further and conducts its search in an increasing orthonormal base. At the first iteration (Fig. 1), the method will normalize the initial guess $\boldsymbol{u}$ and search for the best approximation to the solution that is a scalar multiple of the normalized initial guess vector $\boldsymbol{v}^{(0)}$. At the next iteration, a unit vector $\boldsymbol{v}^{(1)}$, orthogonal to the previous vector, is calculated (using a variation of the Gram–Schmidt technique[5]). The next approximation to the solution is sought in the plane spanned by $\boldsymbol{v}^{(0)}$ and $\boldsymbol{v}^{(1)}$ (Fig. 2). A new vector $\boldsymbol{v}^{(2)}$ is then calculated that is orthogonal to both $\boldsymbol{v}^{(0)}$ and $\boldsymbol{v}^{(1)}$. The search is now conducted in $\boldsymbol{R}^3$. The span of the space in which the search is conducted increases with subsequent iterations.

Another major difference between the two methods is the manner in which the residual vector $\boldsymbol{r}$ is used to influence the search. In

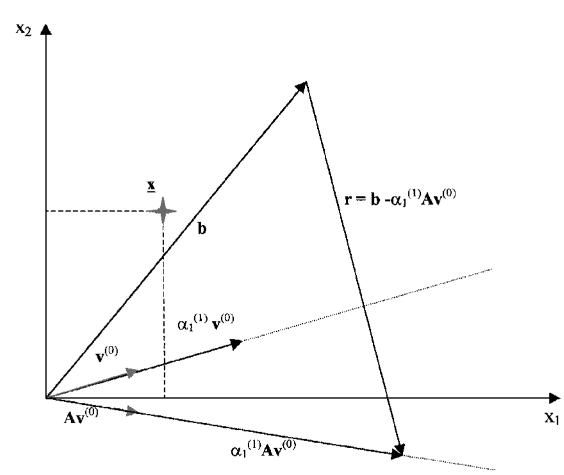

Fig. 1 First iteration of Davidson's method for a system of two equations; $\boldsymbol{v}^{(0)}$ is the normalized initial guess $\boldsymbol{u}$ (not shown).

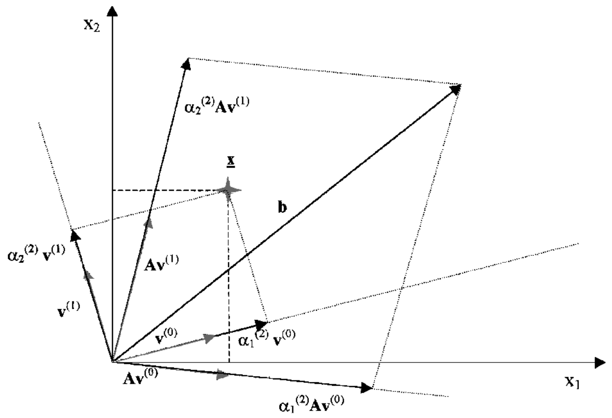

Fig. 2 Second iteration of Davidson's method: sum of the vectors $\alpha_2^{(2)}v^{(1)}$ and $\alpha_1^{(2)}v^{(0)}$ produces a vector that points to the solution.

the CG method, the residual vector is used to define one of the two components of the new search direction. Davidson's method, however, searches through the orthonormal base for the point that will make the length projection of the residual vector onto that base equal to zero. For example, at the first iteration, given a normalized initial guess $\boldsymbol{v}^{(0)}$, a scalar multiple of this vector $\boldsymbol{\alpha}$ is desired such that the product $\boldsymbol{\alpha} \boldsymbol{A}\boldsymbol{v}^{(0)}$ produces a residual vector $\boldsymbol{r}^{(0)}$ with no projection on the direction $\boldsymbol{v}^{(0)}$ (Fig. 1). That is, the inner product

$$\left(\boldsymbol{r}^{(0)}, \boldsymbol{v}^{(0)}\right) = \left(\boldsymbol{b} - \boldsymbol{\alpha} \boldsymbol{A}\boldsymbol{v}^{(0)}, \boldsymbol{v}^{(0)}\right) = 0 \tag{4}$$

This expression can be easily manipulated to obtain an expression for $\boldsymbol{\alpha}$ and also can be stated by saying that the residual vector will have a zero component in the direction of the vector $\boldsymbol{v}^{(0)}$.

For the next iteration, two scalar multiples, α_1 and α_2, will be sought that will make the new residual vector orthogonal to both search directions simultaneously (Fig. 2). This will require solving a pair of simultaneous equations that have the following form:

$$\begin{bmatrix} \left(\boldsymbol{v}^{(0)}, \boldsymbol{A}\boldsymbol{v}^{(0)}\right) & \left(\boldsymbol{v}^{(0)}, \boldsymbol{A}\boldsymbol{v}^{(1)}\right) \\ \left(\boldsymbol{v}^{(1)}, \boldsymbol{A}\boldsymbol{v}^{(0)}\right) & \left(\boldsymbol{v}^{(1)}, \boldsymbol{A}\boldsymbol{v}^{(1)}\right) \end{bmatrix} \begin{bmatrix} \alpha_1 \\ \alpha_2 \end{bmatrix}^{(2)} = \begin{bmatrix} \left(\boldsymbol{v}^{(0)}, \boldsymbol{b}\right) \\ \left(\boldsymbol{v}^{(1)}, \boldsymbol{b}\right) \end{bmatrix} \tag{5}$$

This expression can also be expressed in matrix form. Let the vectors composing the orthonormal base up to and including the current iteration be assembled as the columns of the matrix $\boldsymbol{V}$. The following matrix expression can then be generated:

$$\boldsymbol{V}_{(k,n)}^{T} \boldsymbol{A}_{(n,n)} \boldsymbol{V}_{(n,k)} \boldsymbol{\alpha}_{(k,1)}^{(k)} = \boldsymbol{V}_{(k,n)}^{T} \boldsymbol{b}_{(n,1)} \tag{6}$$

Reducing the Spectral Radius

The convergence rate is drastically improved by reducing the spectral radius. This can be achieved easily; thus, it provides an enormous increase in the convergence rate. The rows of the system are simply divided by the respective diagonal elements of the coefficient matrix. This operation changes the structure of the system and will destroy any symmetry. However, because Davidson's method neither requires nor depends on symmetry to converge, there are no adverse consequences. This operation cannot be performed for the CG method because of the symmetry requirement.

Limiting the Size of the Orthonormal Basis

For extremely large systems of equations, obtaining the components α_i ultimately requires solving extremely large systems of simultaneous equations. This is a potential problem but is overcome easily enough. After m iterations, the matrix containing the orthonormal vectors can be reset. This would take place after calculating the most recent approximation and treating it as the initial guess. The vector would then be normalized, and the corresponding value of $\boldsymbol{\alpha}$ could be calculated that would produce the same vector as the most recent approximation to the solution. For the next iteration, the search for the solution would take place in $\boldsymbol{R}^2$, and iterations can be continued.

The steps of the condensation must be carried out carefully; otherwise, vital information could be lost. An additional benefit of condensing the orthonormal basis after a predetermined number of iterations is that the size of numerous storage arrays can be defined prior to execution of the program, which would otherwise not be possible.

Computational Steps

The following provides a step-by-step description of the program:

1) Set $it = 0$ and $itc = 0$.
2) Obtain an initial guess $\boldsymbol{x}^{(0)}$.
3) $it = it + 1$, and $itc = itc + 1$.
4) Normalize $\boldsymbol{x}^{(0)}$ to obtain $\boldsymbol{v}^{(0)}$ as the first search direction. $\boldsymbol{V}^{(1)}$ consists of $\boldsymbol{v}^{(0)}$. The vectors $\{\boldsymbol{v}^{(0)}, \boldsymbol{v}^{(1)}, \ldots \boldsymbol{v}^{(k-1)}\}$ are stored in the matrix $\boldsymbol{V}^{(k)}$.
5) Calculate and store the vectors $\boldsymbol{A}\boldsymbol{v}^{(k)}$ as the columns of a matrix $\boldsymbol{M}$, $\boldsymbol{A}\boldsymbol{v}^{(0)}$ is stored in $\boldsymbol{M}^{(1)}$ in this case.
6) Calculate the components of the matrix $\boldsymbol{W}^{(k)}$ and the vector $\boldsymbol{B}^{(k)}$ from
   $\boldsymbol{W}^{(k)} = [\boldsymbol{V}^T]^{(k)}[\boldsymbol{A}][\boldsymbol{V}]^{(k)} = [\boldsymbol{V}^T]^{(k)}[\boldsymbol{M}]^{(K)}$
   $\boldsymbol{B}^{(k)} = [\boldsymbol{V}^T]^{(k)}[\boldsymbol{b}]$.
7) Using a direct solver such as Gauss–Jordan elimination, solve the following system of equations for $\boldsymbol{\alpha}^{(k)}$:
   $\boldsymbol{W}^{(k)}\boldsymbol{\alpha}^{(k)} = \boldsymbol{B}^{(k)}$
8) Set $flag = 0$.
9) IF $itc = m$ THEN
   $flag = itc$
   $[\boldsymbol{M}] = [\boldsymbol{M}][\boldsymbol{\alpha}^{(m)}]$
   $[\boldsymbol{W}_{(1,1)}] = [\boldsymbol{\alpha}^T][\boldsymbol{W}][\boldsymbol{\alpha}]$
   $[\boldsymbol{B}_{(1)}] = [\boldsymbol{\alpha}^T][\boldsymbol{B}]$
   $itc = 1$
   END
   IF $flag \neq 0$ THEN
   $\boldsymbol{A}\boldsymbol{x}^{(k)} = 1.0^{*}[\boldsymbol{M}]$
   Go to step #11
   END
10) Calculate the latest approximation to the constant vector using
   $\boldsymbol{A}\boldsymbol{x}^{(k)} = [\boldsymbol{M}^{(k)}][\boldsymbol{\alpha}^{(k)}]$
11) Check whether the convergence criteria have been satisfied using
   $\max|(Ax_i^{(k)} - b_i)/b_i| < \varepsilon$ for $i = 1, 2, \ldots, n$, where ε is the convergence criterion,
   & $flag = 0$, to ensure that condensation is not taking place during this iteration
12) Form the new residual vector direction $\boldsymbol{r}^{(k)}$ from
   $\boldsymbol{y} = (\boldsymbol{A}\boldsymbol{x}_i^{(k)} - \boldsymbol{b}_i)/\boldsymbol{A}_{(i,i)}$ for $i = 1, n$, and
   $\boldsymbol{r}^{(k)} = \boldsymbol{y}/\|\boldsymbol{y}\|$
13) Calculate the vector $\boldsymbol{v}^{(k)}$ that is orthogonal to the base $\boldsymbol{V}^{(k)}$ using the following algorithm for the Gram–Schmidt process:
   $\boldsymbol{y} = \boldsymbol{r}^{(k)}$
   FOR $i = 1, k$
   $\delta = (\boldsymbol{v}^{(i-1)}, \boldsymbol{r}^{(k)})$
   $\boldsymbol{y} = \boldsymbol{y} - \delta \boldsymbol{v}^{(i-1)}$
   $\boldsymbol{y} = \boldsymbol{y}/\|\boldsymbol{y}\|$
   END loop
   $\boldsymbol{v}^{(k-1)} = \boldsymbol{y}$

Table 1 Variables used in program

Symbol	Definition
it	Iteration counter
itc	Internal counter for tracking size of orthonormal base
$\boldsymbol{V}$	Orthonormal base of column vectors
$\boldsymbol{M}$	$[\boldsymbol{A}][\boldsymbol{V}]$
$\boldsymbol{W}$	$[\boldsymbol{V}^T][\boldsymbol{M}]$
$\boldsymbol{B}$	$[\boldsymbol{V}^T][\boldsymbol{b}]$
$\boldsymbol{\alpha}$	Coefficients of unit vectors $\boldsymbol{v}^{(k)}$ approximating the solution
$\boldsymbol{r}$	Residual vector
ε	Convergence criterion

Table 2 Comparison of performance between CG method and Davidson's method

n	c	$A(1,1)$	$A(n,n)$	CG $F(x)$	CG Iter.	Davidson $F(x)$	Davidson Iter.
25	5	115.63	44.99	−5.164804107807360E+04	11	−5.164804107807630E+04	5
25	6	115.63	44.99	−4.813254329786170E+04	11	−4.813254329786540E+04	5
50	8	263.43	99.15	−4.724964225687430E+05	12	−4.724964225681190E+05	4
50	10	263.43	99.15	−4.319308443921390E+05	12	−4.319308443921450E+05	5
50	12	263.43	99.15	−4.025749894361610E+05	12	−4.025749894361660E+05	5
100	15	596.40	220.70	−3.947662073458550E+06	14	−3.947662073455790E+06	4
100	35	596.40	220.70	−3.016404837142820E+06	15	−3.016404837142080E+06	5
150	50	960.70	353.40	−1.083410906665180E+07	16	−1.083410906665080E+07	5
150	98	961.00	353.00	−1.022353967442190E+07	17	−1.022353967441990E+07	6
150	173	961.00	353.00	−1.119892218088950E+07	20	−1.119892218088840E+07	8
200	196	1347.00	494.00	−2.719539763809190E+07	19	−2.719539763808710E+07	7
200	391	1347.00	494.00	−3.953225968473330E+07	32	−3.953225968463580E+07	12
250	307	1751.00	641.00	−5.987506882057660E+07	21	−5.987506882057300E+07	8
250	571	1750.00	640.00	−9.909334646511780E+07	44	−9.909334646500030E+07	17

14) IF $flag = 0$ THEN
    Return to step #3
  ELSE
    $[V_{(i,1)}] = [V^{(m)}][\alpha^{(m)}]$
    $[\alpha^{(1)}] = 1.0$
    Return to step #3
  END

The variables used in the program are defined in Table 1, and a summary of the performances of the two methods is given in Table 2.

Conclusion

Davidson's method is extremely sensitive to roundoff errors and normally will not work properly if single-precision computations are used. It is extremely important that double (or higher) precision be used for this program to function properly. Arbitrary symmetric matrices were used to compare the performance of Davidson's method to the CG method. A simple program was written to construct fairly large symmetric matrices. The diagonal elements are based on the desired size of the matrix. The off-diagonal elements are constants that can be selected by the user.

Table 2 shows a summary of the performances of the two methods: the size of the matrix n, the value of the off-diagonal elements c, and the first and last diagonal elements of the matrix. The next section of Table 2 shows the values of the quadratic function $F(x)$ calculated from the approximate solution along with the number of iterations it took to converge. It is quite apparent from these results that Davidson's method outperforms the CG method as a linear solver.

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Delamination Fracture Toughness of Woven-Fabric Composites Under Mixed-Mode Loading

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Introduction

A NUMBER of composite processing techniques are being developed to reduce manufacturing costs. These techniques include compression molding, resin transfer molding, scrimp, pultrusion, etc. The new processing techniques raise the uncertainty of mechanical properties, particularly the fracture properties. Tension, compression, and shear properties of composites made from various processes were evaluated in Ref. 1. An essential property in the damage tolerance design of laminated composites is the delamination fracture toughness, which is being investigated in this Note. In laminated composite structures, delaminations initiate and propagate under a combination of normal and shear stresses due to either loading or stacking sequence. Therefore, tests of delamination resistance should account for the combined stress state.[2]

The objective of this Note is to evaluate the mode-I, -II, and mixed-mode delamination fracture toughnesses of laminated woven-fabric composites made from autoclave and compression molding processes. An autoclave-molded (ATM) composite provides the baseline data to evaluate compression-molded composites. The compression molding consists of two processes: vacuum-assisted compression molding (CMV) and no-vacuum compression molding (CM). The material used in all processes was high modulus fiber (HMF) 5322/34C carbon/epoxy prepreg. All tests were conducted using split-beam specimen and mixed-mode bending test apparatus.[3]

Material System and Specimen Fabrication

The material used in both the autoclave and compression-molding processes was HMF 5322/34C carbon/epoxy plain-weave prepreg

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