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Perturbation methods for the matrix eigenproblem

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Abstract. Some computational experiments are reported on the solution of the eigenproblem for a matrix **H** by using an iterative sequence of transformations of type $\mathbf{H} \rightarrow \mathbf{S}^{-1}\mathbf{HS}$, where **S** is trivially invertible and is usually calculated from a first-order perturbation formula. Simple improved methods of constructing **S** are reported; these methods greatly improve the convergence properties of the eigenvalue calculations.

1. Introduction

A general principle used in approaching the matrix eigenvalue problem is that an $N \times N$ square matrix **H** and its transform $\mathbf{S}^{-1}\mathbf{HS}$ by a non-singular **S** have the same eigenvalues. A complete diagonalization process seeks to find **S** such that $\mathbf{S}^{-1}\mathbf{HS}$ is diagonal, with **S** containing the eigencolumns. The present note reports some computational experiments which used a more simple form of **S**. This form is obtained by starting from the unit $N \times N$ matrix 1 and then inserting non-zero elements in the Ith column (if the Ith eigenvalue is desired), with the (I, I) element kept equal to 1. Such a matrix takes the form $\mathbf{1}+\mathbf{R}$, where **R** has the property $\mathbf{R}^2 = 0$. It follows that $\mathbf{S} = \mathbf{1}+\mathbf{R}$ has the immediately known inverse $\mathbf{1}-\mathbf{R}$. Such easily-invertible transformations have been used in both time-dependent and time-independent wave operator theory (Jolicard and Billing 1990, 1991). When they are applied to the traditional eigenvalue problem for a square matrix **H** the most simple choice for the non-zero elements in the Ith column of **R** is (in an obvious notation)

$$R(J) = H(I, J)/[H(I, I) - H(J, J)] \tag{1}$$

as given by first-order perturbation theory (Grosjean and Jolicard 1987, Killingbeck 1991). Successive evaluations of $\mathbf{S}^{-1}\mathbf{HS}$ using (1) at each stage modify the elements $H(J, K)$ until **H** finally attains a form with $H(I, I)$ equal to the eigenvalue $E(I)$ and all the other elements $H(J, I)$ equal to zero. Grosjean and Jolicard (1987) applied the procedure to the matrix **H** of the Hamiltonian $-D^2+x^2+\lambda x^4$ set up in a basis of even parity eigenfunctions of $-D^2+x^2$. As λ increases this unperturbed basis becomes more and more unsuitable; the increasing relative magnitude of the off-diagonal matrix elements imposes an increasingly severe test on a formalism using the perturbative prescription (1). Even at $\lambda = 0.2$ Grosjean and Jolicard (1987) found that the process diverges slowly for the ground state ($I = 1$). Our recent computations showed that in such borderline cases the eigenvalue can still be estimated fairly accurately from a Padé approximant analysis of the ultimately divergent sequence of $H(I, I)$ values; however, the sum of the moduli of the elements $H(J, I)$ at first decreases as required

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but then reaches a non-zero minimum and begins to increase again. We report here some simple methods which markedly improve the convergence properties of the process. We note that Kalamboukis (1980) made an analysis of a somewhat similar perturbation prescription which arises in Davidson's method for the matrix eigenproblem.

2. Methods of order N

We call a method of order N one which uses some explicit rule giving each $R(N)$ directly, as does (1); more complicated implicit rules, such as the Gauss–Seidel (GS) one (discussed later) require an amount of computation of order N^2 to produce the column $R(J)$ for each transformation. The two most simple ways to modify the perturbation formula (1), while still only using the matrix elements $H(J, I)$ and the diagonal elements, are as follows.

Method 1. Use (1), but multiply the computed $R(J)$ by a fixed reduction factor β. This simple reduction factor method (RFM) improves the convergence considerably. At $\beta = 1$ convergence for $I = 1$ was not obtained at $\lambda = 0.2$; with $\beta = \frac{1}{2}$ the process converges for $I = 1, 2, 3$ even at $\lambda = 1$, as shown by test calculations on the 20×20 form of H.

Method 2. This method was designed by analogy with the Jacobi transformation method, but uses only one column and will work for non-symmetric **H**; indeed even *if* **H** *is initially symmetric the* **S** *transformations necessarily render it non-symmetric.* This method, to which we have given the name the single-cycle method (SCM), proceeds by using (1) in cyclic fashion. For the case $I = 1$, for example, a sequence of small transformations is applied, in each of which only *one* $R(J)$ is chosen according to (1), with the other $R(J)$ set equal to zero. A complete cycle ($J = 2, 3, \ldots, N$) of such small transformations involves roughly the same total computational effort as one full transformation in which all elements are calculated simultaneously using (1). The subtle new feature which enters is that each small single-element transformation modifies some of the matrix elements involved in the transformation for the next element. This collective effect dramatically improves convergence; even at $\lambda = 2$ (ten times the $I = 1$ limit for the original perturbative formula) the SCM converges at $I = 1, 2$ and 3 for a 50×50 version of the test matrix **H**. Table 1 shows some illustrative results for $\lambda = 0.3$ and $I = 1$ while table 2 shows some specimen SCM results.

3. The Gauss–Seidel approach

Before making each **S** transformation the first-order column estimate (1) can be improved by changing it to a second-order column, using some formalism such as Brillouin–Wigner (BW) perturbation theory. The desired *exact* elements $R(J)$ at each transformation will obey the equation

$$R(J) = \frac{\Sigma_{K \neq J} H(J, K) R(K)}{[E - H(J, J)]} \tag{2}$$

Table 1. The $H(I, I)$ sequence for the 20×20 version of **H** at $\lambda = 0.3$. $I = 1$. NI is the iteration number and both RFM and SCM results are shown.

NI	$\beta = 1$	$\beta = 0.7$	SCM
2	1.172 008 131	1.170 417 312	1.163 564 807
4	1.167 160 166	1.165 398 998	1.163 975 214
6	1.165 977 236	1.164 413 503	1.164 038 328
8	1.165 577 253	1.164 162 477	1.164 045 989
10	1.165 464 158	1.164 088 019	1.164 046 982
12	1.165 514 277	1.164 063 241	1.164 047 126
14	1.165 702 893	1.164 054 121	1.164 047 151
16	1.166 050 331	1.164 050 434	1.164 047 156
18	1.166 614 693	1.164 048 808	1.164 047 157
20	1.167 502 973	1.164 048 034	1.164 047 157

where the $H(J, K)$ are the current elements in the transformed **H** matrix; use of these exact elements would finish the calculation in one step. In practice only an approximate set of $R(J)$ can be calculated, so that several iterations will be required. The equations (2) can be used in several ways in approximate calculations, and two different uses seem to be confused in the terminology used by Arias de Saavedra and Buendia (1991). In their work, of course, **H** is fixed throughout, so that the $R(J)$ in (2) are interpreted directly as eigencolumn elements; this does not affect the general principles involved. Two principal modes of use of (2) are as follows.

The BW *mode.* $R(I)$ is set equal to 1, with all other $R(J)$ zero. The quantities on the right of (2) are all worked out for the *current* $R(J)$ (using some trial E value) and are held in a temporary array $T(J)$ before being finally copied back into the $R(J)$ array. Applying this process M times gives the provisional Brillouin-Wigner eigencolumn. To fix the value of E this column is substituted in the eigenvalue equation

$$E = H(I, I) + \sum_{J \neq I} H(I, J)R(J) \tag{3}$$

and the whole process is iterated to self-consistency (for a fixed order M).

The GS *mode.* In this mode equations (2) and (3) are applied repetitively in an attempt to obtain convergence; the vital difference from the BW mode is that the $R(J)$ are *not* initialized again to the value zero or unity at the start of each cycle. This direct process was actually used effectively by Fernandez *et al* (1985) for the same kind of two-dimensional perturbed oscillator problem treated in a hybrid manner by Arias de

Table 2. Converged $H(I, I)$ values for the 60×60 version of **H**. The results agree with the eigenvalues given by the hypervirial perturbation method (Killingbeck 1991).

λ	$I = 1$	$I = 2$	$I = 3$
0.5	1.241 854 060	7.396 900 639	15.136 845 75
1.0	1.392 351 642	8.655 049 958	18.057 557 44
1.5	1.509 415 693	9.591 537 272	20.193 182 55
2.0	1.607 541 302	10.358 583 38	21.927 166 19

Saavedra and Buendia (1991). The latter authors calculated the eigenvalue from a Rayleigh quotient based on what they termed a BW column, although it was actually found by using (2) in GS mode. The work of Fernandez *et al* (1985) indicates that the GS mode is often adequate to give the eigenvalue on its own without any subsidiary calculations.

The difference between the BW and GS modes can be described and illustrated clearly for our test matrix. If the BW calculation for the state $I=1$ is taken to third order, it will produce non-zero values for the $R(J)$ up to $J=7$, together with an approximate eigenvalue. However, if the GS mode is used, including coefficients up to $R(7)$, the result is the lowest eigenvalue in the subspace spanned by the seven bias states. Table 3 shows quite clearly the difference between the rates of convergence of the two approaches as the order M increases. The BW approach only uses information about selected combinations of the matrix elements, whereas the GS approach freely uses all of the matrix elements within the coupled subspace activated at a particular order M.

Table 3. Comparison of Brillouin-Wigner and Gauss-Seidel eigenvalues for increasing perturbation order M, with $I=1$ and $\lambda=0.1$.

M	BW	GS
0	1.075	1.075
1	1.064 473 680	1.065 375 667
2	1.065 636 975	1.065 285 701
3	1.065 187 287	1.065 285 510
4	1.065 329 191	1.065 285 510
12	1.065 285 946	1.065 285 510
13	1.065 285 204	1.065 285 510

In the above BW and GS calculations the matrix **H** was held fixed throughout. We have also performed some computations in which one or more cycles of the GS iteration are performed to produce the $R(J)$ for each **S** transformations. The two methods then operate in a symbiotic manner; the GS iteration gives an $R(J)$ column of reasonable accuracy for the **S** transformation, while the **S** transformation reduces the size of the elements $H(J, I)$, assisting in the convergence of the GS process. For example, for a 20×20 version of H, with $\lambda=0.5$, 50 cycles of a combined process gave the $I=3$ eigenvalue 15.136 845 76. At $\lambda=1$, 120 cycles gave the $I=3$ eigenvalue 18.057 557 44. The Gauss-Seidel iterative approach used alone took 150 cycles for the $\lambda=0.5$ case and diverged for the $\lambda=1$ case. Each cycle of the combined calculation began with zero values for all $R(J)$ except $R(I)$, although the column calculating according to (1) could be used. Two cycles of Gauss-Seidel iteration were used, followed by an S transformation. Even the use of the simple starting column with one Gauss-Seidel iteration gives better convergence properties than the use of equation (1) alone, since the $R(J)$ with high J values are effectively of high perturbation order rather than of first order. Preliminary results suggest that the GS approach to calculating the $R(J)$ column is roughly as effective as the SCM at producing convergence of the **S** transformation method, although the SCM is more simple for computer programming.

Each element $X(J)$ of the desired eigencolumn of the matrix **H** is found very simply in the **S** transformation method. It is given by the sum of the $R(J)$ values used in the

sequence of transformations which bring **H** to reduced form (which form, incidentally, provides a matrix of dimension reduced by one and with all the eigenvalues of **H** except one). The successively augmented $X(J)$ values thus resemble the partial sums of a series, with the $R(J)$ being the terms in the series. Padé analysis or simple Aitken extrapolation of the sequence of $H(I, I)$ values gives a good eigenvalue estimate before the $H(I, I)$ sequence has converged. The interesting possibility arises that some form of extrapolation process on the sequence of successive $R(J)$ column elements might provide a method for accelerating the convergence of the **S** transformation method; this possibility is currently being investigated. The principal emphasis in the calculations reported here was on obtaining convergence; for our test problem a few hundred iterations may be necessary for $I = 3$ and a large λ value.

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