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An Iterative Procedure for the Calculation of the Lowest Real Eigenvalue and Eigenvector of a Nonsymmetric Matrix

A new and promising method for the calculation of electronic wavefunctions of atoms and molecules [1] involves in some of its steps the calculation of the lowest eigenvalue and corresponding eigenvector of an almost-symmetric matrix. Although a few, very efficient, procedures are available for the general non-symmetric eigenvalue problem [2, 3], there have been no effective methods which are specifically tailored for the calculation of the lowest root only, particularly for the case in which the matrix has a strongly dominant main diagonal and in which a reasonable initial guess can be provided for the left- and right-eigenvectors.

A very effective solution for the symmetric analogue of this problem by an iterative technique has been given by Nesbet [4], and the aim of the present note is to show that this technique can be extended to the nonsymmetric case. A modification of Nesbet's algorithm, devised by one of the present authors [5] in order to facilitate efficient application to very large and/or sparse matrices, can also be extended to the nonsymmetric case. As in Nesbet's original method, the computational effort is roughly proportional to the square of the dimension of the matrix; in the modified form for sparse matrices the effort is approximately proportional to the number of non-zero matrix elements only.

As in the original procedure, the algorithm will be developed for the generalized eigenvalue problem,

$$\mathbf{Hc} = E\mathbf{Sc}, \tag{1}$$

where $\mathbf{H}$ is the given real non-symmetric matrix, $\mathbf{S}$ is a given metric ("overlap matrix") which is real and positive definite (in most cases $\mathbf{S}$ is just the unit matrix), E is the desired real eigenvalue, and $\mathbf{c}$ is the corresponding right-eigenvector. The left-eigenvector $\mathbf{b}$ belonging to E satisfies the equation

$$\mathbf{b}^T\mathbf{H} = E\mathbf{b}^T\mathbf{S}, \tag{2}$$

where the superscript T denotes the transpose. (The eigenvalue E is real if $\mathbf{H}$ is not very "far" from symmetric and if the eigenvalue of $\frac{1}{2}(\mathbf{H} + \mathbf{H}^T)$ which is closest to E is nondegenerate and well separated; for if E is complex, then E^* would

also be an eigenvalue of $\mathbf{H}$, and this pair of complex eigenvalues would coalesce to a degenerate eigenvalue of $\frac{1}{2}(\mathbf{H} + \mathbf{H}^T)$ in the limit as $\mathbf{H} - \mathbf{H}^T \to \mathbf{0}$.)

Given some estimates $\mathbf{c}$ and $\mathbf{b}$ for the right- and left-eigenvectors, respectively, a corresponding estimate for the eigenvalue (analogous to Eq. (2–4) of [5]) would be obtained from

$$E = \mathbf{b}^T\mathbf{H}\mathbf{c}/(\mathbf{b}^T\mathbf{S}\mathbf{c}). \tag{3}$$

If the errors in $\mathbf{b}$ and $\mathbf{c}$ are of order ϵ, then the error in E would be of order ϵ^2, since terms such as $\boldsymbol{\epsilon}^T\mathbf{H}\mathbf{c}$ and $\mathbf{b}^T\mathbf{H}\boldsymbol{\epsilon}$ reduce to $E\boldsymbol{\epsilon}^T\mathbf{S}\mathbf{c}$ and $E\mathbf{b}^T\mathbf{S}\boldsymbol{\epsilon}$, respectively, when $\mathbf{b}$ and $\mathbf{c}$ are the appropriate exact eigenvectors. Proceeding as in Ref. [5], Eq. (5–9), the μ-th elements of $\mathbf{b}$ and $\mathbf{c}$ are modified according to the sequence of steps:

$$f_\mu = \sum_{\lambda=1}^{n} S_{\mu\lambda}c_\lambda\,, \tag{4}$$

$$f_\mu' = \sum_{\lambda=1}^{n} b_\lambda S_{\lambda\mu}\,, \tag{5}$$

$$\sigma_\mu = \sum_{\lambda=1}^{n} H_{\mu\lambda}c_\lambda - Ef_\mu\,, \tag{6}$$

$$\sigma_\mu' = \sum_{\lambda=1}^{n} b_\lambda H_{\lambda\mu} - Ef_\mu'\,, \tag{7}$$

$$\Delta c_\mu = \sigma_\mu/(ES_{\mu\mu} - H_{\mu\mu}), \tag{8}$$

$$\Delta b_\mu = \sigma_\mu'/(ES_{\mu\mu} - H_{\mu\mu}), \tag{9}$$

$$\Delta D = (\Delta b_\mu)f_\mu + f_\mu'(\Delta c_\mu) + (\Delta b_\mu)\,S_{\mu\mu}(\Delta c_\mu), \tag{10}$$

$$\Delta E = (\Delta b_\mu)\,\sigma_\mu/(D + \Delta D) = \sigma_\mu'(\Delta c_\mu)/(D + \Delta D), \tag{11}$$

with b_μ, c_μ, D, and E being adjusted by the appropriate increments at the end of this process. Keeping one component of $\mathbf{b}$ and $\mathbf{c}$ fixed (this would preferably be the dominant component—see the discussion of convergence in Ref. [5]), all other components are adjusted repeatedly in any sequence, until all the Δb_μ and Δc_μ for a complete cycle over μ are smaller in magnitude than a specified criterion C. At this time the iterations are complete and the error in E is of order C^2.

A Fortran program for this procedure in the special case of $\mathbf{S} = \mathbf{1}$ is available upon request from the authors.

If the matrix is too large to fit into the central store of the computer as an ordinary two-dimensional array, or if advantage is to be taken of considerable sparsity in $\mathbf{H}$ (and $\mathbf{S}$), then a procedure similar to that presented in [5] for large

and/or sparse matrices can be applied. The detailed procedure would then consist of the following sequence of steps (the reverse arrow $\leftarrow$ denotes replacement):

I. *Initialization*

1. Obtain an initial approximation for **b** and **c** (e.g., $b_\nu = c_\nu = 1$ for the dominant component and $b_\mu = c_\mu = 0$ for all $\mu \neq \nu$).
2. Set $\mathbf{t} = \mathbf{u} = \mathbf{0}$ (two n-dimensional vectors).
3. For $\mu = 1, 2, \ldots, n$, in turn:
   (a) Obtain row μ ($S_{\mu\lambda}$ and $H_{\mu\lambda}$ for $\lambda = 1, 2, \ldots, n$).
   (b) For each $\lambda = 1, 2, \ldots, n$ set $t_\lambda \leftarrow t_\lambda + b_\mu S_{\mu\lambda}$ and $u_\lambda \leftarrow u_\lambda + b_\mu H_{\mu\lambda}$.
4. Compute $D = \sum_\mu t_\mu c_\mu$, $N = \sum_\mu u_\mu c_\mu$, $E = N/D$.

II. *Iteration*

1. Set $\Delta c_{\max} = 0$.
2. For each $\mu = 1, 2, \ldots, n$, except $\mu = \nu$ (the fixed component):
   (a) Obtain row μ.
   (b) Compute $f_\mu = \sum_{\lambda=1}^{n} S_{\mu\lambda} c_\lambda$ and $g_\mu = \sum_{\lambda=1}^{n} H_{\mu\lambda} c_\lambda$.
   (c) Compute $\sigma_\mu = g_\mu - E f_\mu$ and $\sigma_\mu' = u_\mu - E t_\mu$.
   (d) Compute $\Delta c_\mu = \sigma_\mu/(E S_{\mu\mu} - H_{\mu\mu})$ and $\Delta b_\mu = \sigma_\mu'/(E S_{\mu\mu} - H_{\mu\mu})$.
   (e) Set $D \leftarrow D + \Delta b_\mu f_\mu + t_\mu \Delta c_\mu + \Delta b_\mu S_{\mu\mu} \Delta c_\mu$.
   (f) Set $E \leftarrow E + \sigma_\mu' \Delta c_\mu/D$.
   (g) Set $c_\mu \leftarrow c_\mu + \Delta c_\mu$, $b_\mu \leftarrow b_\mu + \Delta b_\mu$, and $\Delta c_{\max} \leftarrow \max(\Delta c_{\max}, |\Delta c_\mu|, |\Delta b_\mu|)$.
   (h) For each $\lambda = 1, 2, \ldots, n$, set $t_\lambda \leftarrow t_\lambda + \Delta b_\mu S_{\mu\lambda}$ and $u_\lambda \leftarrow u_\lambda + \Delta b_\mu H_{\mu\lambda}$.
3. If $\Delta c_{\max} > C$ (at the end of a complete iteration), repeat from Step II.1.

If the word length of the computer is rather short and there is danger of excessive accumulation of round-off errors in the continuous updating of **t** and **u** in Step II.2(h), then new sums as in Step I.3(b) should be accumulated during each iteration, separately from the current updating in Step II.2(h), and substituted for the latter updated values at the end of each complete iteration. Similarly, round-off error accumulation in the continuous updating of D and E can be reduced by recalculating these quantities at the end of each iteration (or only after the last iteration) as in Step I.4. For the case of $\mathbf{S} = \mathbf{1}$ all the steps involving **S** would be omitted, replacing f_μ, t_μ, and $S_{\mu\mu}$ by c_μ, b_μ and 1, respectively.

The handling of sparse matrices is analogous to the case of symmetric matrices

discussed in [5]. The convergence properties are also similar to those in the symmetric case, and depend upon the dominance of the main diagonal of $\mathbf{H} - E\mathbf{S}$ and upon the eigenvalue E (and its approximations throughout the iterations) being well-separated from the values of $H_{\mu\mu}/S_{\mu\mu}$ for all $\mu \neq \nu$ (where c_ν and b_ν are the fixed components of $\mathbf{c}$ and $\mathbf{b}$, respectively). It has also been found in many test calculations that for almost-symmetric matrices the right-eigenvector approximation $\mathbf{c}$ can be used for $\mathbf{b}$ as well throughout the iterations without serious effect on convergence qualities; in numerous calculations with $n = 10$ to $n = 100$, convergence was generally obtained in fewer than 10 iterations even with this further approximation.

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