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Note

A New Iterative Method for Solution of a Large-Scale General Eigenvalue Problem

The finite-element method is a powerful tool for numerical analysis of an oscillation of a geometrically or physically complicated object such as an analysis of MHD spectra of a cylindrical or toroidal plasma [1–3]. This analysis requires the solution of a large-scale general eigenvalue problem of matrices, $A\mathbf{X} = \lambda B\mathbf{X}$, where matrices A and B are assembled from coefficients of bilinear forms of plasma displacements corresponding to the potential and kinetic energies, respectively. Matrix A is real symmetric or Hermitian, and matrix B is positive definite; moreover, as a consequence of the finite-element formulation they are sparse band matrices.

Many kinds of algorithms for solving a standard eigenvalue problem, i.e., $A\mathbf{X} = \lambda\mathbf{X}$, are now available [4]. Especially if the matrix A is a sparse band matrix, the eigenvalue problem of a very large matrix, e.g., several thousand to several ten thousand dimensional, can be solved. However, there are only a small number of available algorithms for the calculation of a general eigenvalue problem of large-scale matrices. One of the most important things to be noted in solving a large-scale problem is that one should conserve the sparseness of the matrices during the course of the calculation. From this point of view, inverse power methods [5–7] and power methods [8] are considered to be the most favorable methods for solving a general eigenvalue problem.

Here we present a new iterative method for solving the problem, by which we reduce the general to a standard eigenvalue problem without destroying the band structure of the matrices and then we obtain the arbitrary eigenvalue by using an appropriate algorithm for the calculation of the standard eigenvalue problem. This method concerns only the procedure of converting a general to a standard eigenvalue problem, and it will manifest its effectiveness if one can use a most appropriate algorithm to solve the standard eigenvalue problem for each general eigenvalue problem considered.

When one wishes to solve a large-scale eigenvalue problem it is often the case that only a small number of eigenvalues and eigenvectors are necessary. If the jth eigenvalue ($\lambda^j, j = 1, 2,..., N$) and the corresponding eigenvector ($\mathbf{X}^j, j = 1, 2,..., N$) of the general eigenvalue problem ($A\mathbf{X} = \lambda B\mathbf{X}$) of $N \times N$ matrices A and B are required, they will be obtained according to the following procedure.

(1) Prepare an arbitrary initial value ($\lambda_1{}^j$) for the jth eigenvalue (λ^j).

(2) In the nth step of the iteration scheme, shift the eigenvalue by $\lambda_n{}^j$; then the problem is reduced to

$$U_n{}^j\mathbf{X}_n{}^j = (\lambda^j - \lambda_n{}^j)\, B\mathbf{X}_n{}^j, \tag{1}$$

where

$$U_n{}^j = A - \lambda_n{}^j B. \tag{2}$$

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(3) Approximate the above general eigenvalue problem (Eq. (1)) by the standard eigenvalue problem

$$U_n{}^j \mathbf{X}_n{}^j = \Delta\lambda_n{}^j \mathbf{X}_n{}^j \tag{3}$$

and solve it.

(4) If the jth eigenvalue $\Delta\lambda_n{}^j$ of the above standard eigenvalue problem is sufficiently small, i.e., $| \Delta\lambda_n{}^j |/| \lambda_n{}^j | < \epsilon$, then stop the iteration and calculate the corresponding eigenvector $(\mathbf{X}_n{}^j)$.

(5) Calculate a new eigenvalue $\lambda_j^{n+1} = \lambda_n{}^j + \Delta\lambda_n{}^j$ for the next step and return to process (2).

By using an appropriate algorithm for the solution of the standard eigenvalue problem in process (3) one can keep the bandwidth of the relevant matrices constant throughout the above procedure.

For practical use we normalize the eigenvalue so that the norm of matrix B is nearly unity, and then we accelerate the convergence of the iteration. In our procedure we normalize the eigenvalues by the factor $\beta = N/\sum_{i=1}^{N} | B_{ii} |$, instead of calculating the norm of matrix B exactly, and reduce the eigenvalue problem to

$$A\mathbf{X} = \tilde{\lambda}\tilde{B}\mathbf{X}, \tag{4}$$

where $\tilde{\lambda} = \lambda/\beta$, and $\tilde{B} = \beta B$. Then an accelerating coefficient $\omega_n{}^j$ is introduced which is multiplied to $\Delta\lambda_n{}^j$ in each step of the iteration, and the equation of process (5) is replaced by

$$\tilde{\lambda}_{n+1}^j = \tilde{\lambda}_n{}^j + \omega_n{}^j \Delta\tilde{\lambda}_n{}^j. \tag{5}$$

The value of the accelerating coefficient $\omega_n{}^j$ is asymptotically determined by the ratio of Rayleigh quotients of Eqs. (1) and (3) as

$$\omega_n{}^j \xrightarrow[n\to\infty]{} \frac{\| \mathbf{X}^j \|^2}{(\mathbf{X}^j, B\mathbf{X}^j)}, \tag{6}$$

where $\mathbf{X}^j$ is the jth eigenvector of the original problem. Obvioulsy the above asymptotic accelerating coefficient can be calculated only after the convergence of the iteration and, therefore, we cannot determine the value of the accelerating coefficient from Eq. (6) for practical purposes. We adopt the values determined according to the following empirically derived rule.

(1) When the sequence of eigenvalues is monotonic in the vicinity of the nth step of the iteration,[1] that is, $\lambda_n{}^j < \lambda_{n-1}^j < \lambda_{n-2}^j$ or $\lambda_n{}^j > \lambda_{n-1}^j > \lambda_{n-2}^j$,

$$\begin{aligned} \omega_n{}^j &= 2\omega_{n-1}^j, \qquad \text{for} \quad \omega_{n-1}^j \leqslant 5, \\ &= 10, \qquad\quad \text{for} \quad \omega_{n-1}^j > 5. \end{aligned} \tag{7}$$

[1] As we prove below, the sequence of the eigenvalues monotonically increases if the iteration is not accelerated. But by the acceleration the monotonicity is destroyed, and the sequence can become oscillatory locally.

(2) When the sequence of eigenvalues is oscillatory in the vicinity of the nth step of the iteration, that is, $\lambda_{n-1}^j < \lambda_n{}^j < \lambda_{n-2}^j$ or $\lambda_{n-1}^j > \lambda_n{}^j > \lambda_{n-2}^j$,

$$\begin{aligned} \omega_n{}^j &= \omega_{n-1}^j/4, \qquad \text{for} \quad \omega_{n-1}^j \geqslant 4, \\ &= 1, \qquad\quad\ \text{for} \quad \omega_{n-1}^j < 4. \end{aligned} \tag{8}$$

By means of the above rule the iteration is accelerated sufficiently, as shown below.

In order to prove the convergence of the procedure we consider the following situation: (1) A is real symmetric or Hermitian, and B is real symmetric; (2) B is a positive definite matrix, and

$$\max_{\mathbf{X}} \frac{(B\mathbf{X}, \mathbf{X})}{\| \mathbf{X} \|^2} < 1. \tag{9}$$

In the following we prove the convergence of the procedure as for the minimum eigenvalue (λ^1).[2] It should also be remarked that, for simplicity, the acceleration process described above is not taken into account. By the iterative procedure the approximate eigenvalue for each step constitutes an infinite sequence ($\lambda_1{}^1, \lambda_2{}^1, \ldots$). First, we prove that this sequence is monotonically increasing and uniformly bounded. For an arbitrarily chosen scalar α which satisfies $\alpha < \lambda^1$, we define a matrix $U_\alpha \equiv A - \alpha B$ and represent the minimum eigenvalue of the matrix U_α by $\Delta\alpha$, that is,

$$\Delta\alpha = \min_{\mathbf{X}} \frac{((A - \alpha B)\,\mathbf{X}, \mathbf{X})}{\| \mathbf{X} \|^2}. \tag{10}$$

Because the vector $U_\alpha \mathbf{X}$ can be decomposed as

$$U_\alpha \mathbf{X} = (A - \alpha B)\mathbf{X} = (A - \lambda^1 B)\mathbf{X} + (\lambda^1 - \alpha)\, B\mathbf{X}, \tag{11}$$

the following inequality is derived,

$$\Delta\alpha \geqslant \min_{\mathbf{X}} \frac{((A - \lambda^1 B)\,\mathbf{X}, \mathbf{X})}{\| \mathbf{X} \|^2} + \min_{\mathbf{X}} \frac{(\lambda^1 - \alpha)(B\mathbf{X}, \mathbf{X})}{\| \mathbf{X} \|^2}. \tag{12}$$

As λ^1 is the eigenvalue of the problem $A\mathbf{X} = \lambda B\mathbf{X}$, and B is positive definite,

$$\min_{\mathbf{X}} \frac{((A - \lambda^1 B)\,\mathbf{X}, \mathbf{X})}{\| \mathbf{X} \|^2} = 0, \tag{13}$$

[2] The proof is easily generalized for the convergence of the iteration for the other eigenvalues by using the following definition for $\Delta\alpha$,

$$\Delta\alpha = \min_{E_j} \max_{\mathbf{X} \in E_j} \frac{((A - \alpha B)\mathbf{X}, \mathbf{X})}{\| \mathbf{X} \|^2} \qquad (j = 2, 3, \ldots, N),$$

where E_j is a j-dimensional subspace of the original N-dimensional space.

and

$$\min_{\mathbf{X}} \frac{(B\mathbf{X}, \mathbf{X})}{\| \mathbf{X} \|^2} > 0. \tag{14}$$

Therefore, $\Delta\alpha$ is always positive, and thus $\alpha < \alpha + \Delta\alpha$. Using Eqs. (11) and (13), we obtain

$$\lambda^1 - \alpha = \min_{\mathbf{X}} \frac{((A - \alpha B)\,\mathbf{X}, \mathbf{X})}{(B\mathbf{X}, \mathbf{X})}. \tag{15}$$

From Eqs. (9) and (15) the following inequality is derived.

$$\lambda^1 - \alpha > \min_{\mathbf{X}} \frac{((A - \alpha B)\,\mathbf{X}, \mathbf{X})}{\| \mathbf{X} \|^2} = \Delta\alpha. \tag{16}$$

Therefore, $\alpha + \Delta\alpha < \lambda^1$ for $\alpha < \lambda^1$, that is, the infinite sqeuence $(\lambda_1{}^1, \lambda_2{}^1, \ldots)$ is monotonically increasing and uniformly bounded. Next, we prove that λ^1 is the limit of the sequence. We assume that the value of the limit is less than λ^1, that is,

$$\lim_{n\to\infty} \lambda_n{}^1 = \bar{\lambda} < \lambda^1. \tag{17}$$

Then we substitute $\bar{\lambda}$ for α in the definition of the matrix U_α. As a consequence of the above discussion there exists $\bar{\lambda}' = \alpha + \Delta\alpha > \bar{\lambda}$, which is inconsistent with the above assumption (Eq. (17)). Therefore, it is proved that λ^1 is the limit of the infinite sequence $(\lambda_1{}^1, \lambda_2{}^1, \ldots)$.

To investigate the accuracy and convergence of the procedure we solved a general eigenvalue problem with rather small-scale matrices ($N = 41$ and the band width $= 6$), which appears in the analysis of the MHD spectra of a current carrying cylindrical plasma [1]. In this case eigenvalues represent squared frequencies of the MHD oscillation, and the growth rate of the instability is given by the square root of the absolute value of a negative eigenvalue. Figure 1 shows that oscillations corresponding to the three lowest eigenvalues (Nos. 1, 2, and 3) are unstable and that those corresponding to the fourth and higher eigenvalues are stable. It is easily seen from this figure that results with an accuracy of 10^{-3} are attained within several iterations and that the stopping criterion ($| \Delta\lambda_n{}^j | / | \lambda_n{}^j | < \epsilon$; $\epsilon = 10^{-4}$) is satisfied within about 10 iterations. Another remarkable point of this procedure is that the result is insensitive to the initial trial values of the eigenvalue and roughly approximated values are usually obtained after the first or second iteration (Fig. 2). In this example three different initial trial values are chosen for the lowest eigenvalue, and all the initial trial values give almost same results within an accuracy range of 10^{-3} at the second step of the iteration.

In summary, there are two remarkable features and some problems to be solved in the new algorithms. Namely,

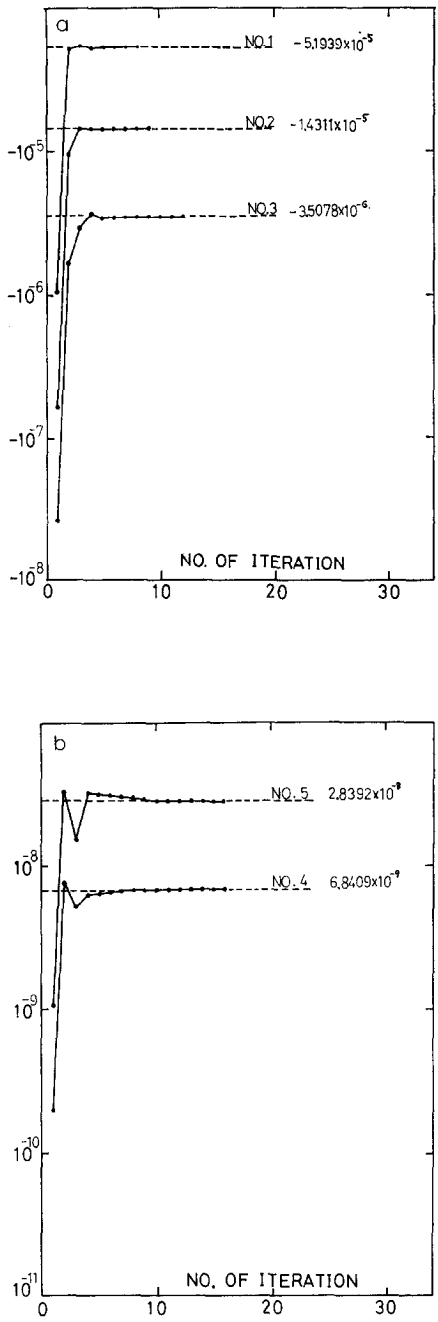

FIG. 1. An example of a solution of a general eigenvalue problem which appears in an analysis of MHD oscillations of a current carrying cylindrical plasma. (a) Eigenvalues corresponding to unstable modes. (b) Eigenvalues corresponding to the lowest two stable modes.

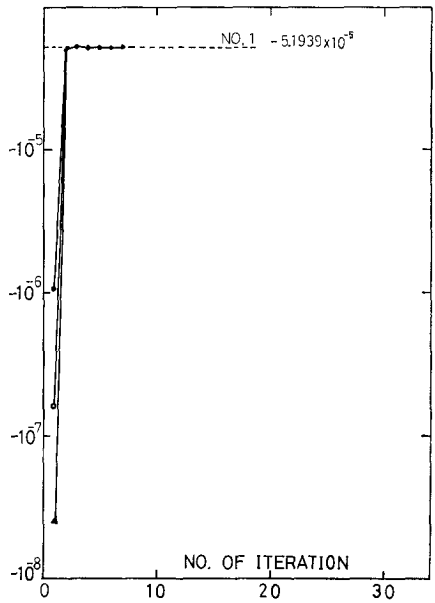

FIG. 2. Processes of convergence for different values of initial guesses.

(1) The band structure or sparseness of the original matrices is conserved during the course of reducing the general eigenvalue problem to a standard eigenvalue problem. This is one of the most attractive points of the method when one wishes to solve a large-scale general eigenvalue problem.

(2) The results are insensitive to the choice of initial trial values of an eigenvalue, and one can reach a desired eigenvalue by always choosing the eigenvalue of the same number counted from the lowest eigenvalue at each step of the iteration scheme.

(3) This procedure works very well for solving a general eigenvalue problem as long as a suitable algorithm for a standard eigenvalue problem is available. Therefore, it is very important to find a most adequate algorithm for the standard eigenvalue problem.

(4) Problems concerning degenerate eigenvalues have not been studied yet. For such problems, the proof of convergence presented in this paper, at least, should be reexamined.

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