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Chapter 19

CONVERGENCE OF SUBSPACE ITERATION

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Abstract

The convergence of subspace iteration for the solution of eigenpairs is studied. The theoretical convergence rate is derived and is presented with emphasis on the theory in the light of practical implications. Various techniques to accelerate the convergence of the subspace iterations are proposed and are tested in a preliminary manner on some demonstrative sample problems.

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1. Introduction

During recent years the development of solution techniques for calculating the eigensystem of large eigenproblems has attracted an increasing amount of attention [1-3]. A particularly important eigenproblem encountered in computational mechanics is the calculation of some eigenpairs of the generalized eigenproblem

$$\underline{K}\underline{\varphi} = \lambda \underline{M}\underline{\varphi} \ , \qquad (1)$$

where $\underline{K}$ and $\underline{M}$ are the stiffness and mass matrices of the discrete degree of freedom system, and $(\lambda_i, \underline{\varphi}_i)$ is the i'th eigenpair. If the order of $\underline{K}$ and $\underline{M}$ is n, we have n eigenpairs which we order as follows,

$$\begin{gathered} \lambda_1 \le \lambda_2 \le \lambda_3 \le \cdots \le \lambda_n \\ \underline{\varphi}_1 \, ; \, \underline{\varphi}_2 \, ; \, \underline{\varphi}_3 \, ; \, \cdots \, ; \, \underline{\varphi}_n \ . \end{gathered} \qquad (2)$$

Thus, the solution for p eigenvalues and corresponding eigenvectors can be written as

$$\underline{K}\underline{\Phi} = \underline{M}\underline{\Phi}\underline{\Lambda} \quad (3)$$

where the columns of $\underline{\Phi}$ store the eigenvectors and $\underline{\Lambda}$ is a diagonal matrix with the eigenvalues on the diagonal.

Among the techniques for calculating the lowest eigenvalues and corresponding eigenvectors of Eq. (1), the subspace iteration method has found increasing use [1, 4-6]. The subspace iteration method has been applied successfully to the solution of a large number of problems and Table 1 summarizes some typical solution times. In previous publications, the basic equations of the method have been presented, and the practical implementation was discussed [4, 7], but no detailed discussion of the convergence of the subspace iteration method was given. However, for the practical use of the technique and in the search for methods to increase the effectiveness of the basic algorithm, it is important to have sufficient insight into the convergence characteristics.

Table 1 Solution Times Using Subspace Iteration Method

System	System order	Maximum half band-width	Mass matrix	Number of eigen-pairs	Com-puter used	Central proces-sor sec.
Wind-tunnel	5952	215	Diagonal	10	CDC 7600	1000
Dam	2916	491	Diagonal	4	CDC 7600	495
Instru-ment cabinet	10456	548	Diagonal	20 (9)	CDC 7600	3921 (1036)
Insula-tion frame-work	1965	221	Diagonal	25	CDC 7600	192

The objective of this paper is to discuss in detail the convergence properties of the subspace iteration method with specific emphasis on presenting the theory in the light of practical implications. First, in the paper, the basic equations that are solved in subspace iteration are briefly summarized, and the importance of each equation solved is explained. Emphasis is placed to show in detail how the minimization of the Rayleigh quotient is used to extract the best eigenvalue and eigenvector approximations from the current subspace. In the next part of the paper the proof for the ultimate convergence rate is given, and relevant practical consequences are discussed. A particularly important phase of the subspace iteration method is the selection of an effective starting subspace. In the paper, the starting subspace that has been found effective is described in detail together with various recent experiences gathered. Also, a number of techniques to accelerate the convergence of the subspace iterations are proposed.

2. The Subspace Iteration Method

Assume in the following that the order of the matrices $\underline{K}$ and $\underline{M}$ in Eq. (1) is n and that we require the lowest p eigenvalues and corresponding eigenvectors. The subspace iteration solution consists of the following three steps:

(1) Establish q starting iteration vectors, $q > p$, which span the starting subspace E_1.

(2) Perform subspace iterations, in which simultaneous inverse iteration is used on the q vectors, and Ritz analysis is employed to extract optimum eigenvalue and eigenvector approximations at the end of each inverse iteration.

(3) After iteration convergence, use the Sturm sequence check to verify that the required eigenvalues and corresponding eigenvectors have been calculated.

The verification of the solution results in step (3) is straightforward and is discussed in detail in [7]. The effectiveness of the algorithm lies in the procedures used in steps (1) and (2).

Assume that we have established the q starting iteration vectors, in $\underline{X}_1$, *then the subspace iteration in (2) is as follows:*

For $k = 1, 2, \ldots$, iterate from subspace E_k to subspace E_{k+1}:

$$\underline{K}\bar{\underline{X}}_{k+1} = \underline{M}\underline{X}_k \quad . \tag{4}$$

Calculate the projections of the matrices $\underline{K}$ and $\underline{M}$ onto E_{k+1}:

$$\underline{K}_{k+1} = \bar{\underline{X}}_{k+1}^T \underline{K}\bar{\underline{X}}_{k+1} \tag{5}$$

$$\underline{M}_{k+1} = \bar{\underline{X}}_{k+1}^T \underline{M}\bar{\underline{X}}_{k+1} \quad . \tag{6}$$

Solve for the eigensystem of the projected matrices:

$$\underline{K}_{k+1}\underline{Q}_{k+1} = \underline{M}_{k+1}\underline{Q}_{k+1}\underline{\Lambda}_{k+1} \quad . \tag{7}$$

Calculate an improved approximation to the eigenvectors:

$$\underline{X}_{k+1} = \bar{\underline{X}}_{k+1}\underline{Q}_{k+1} \quad . \tag{8}$$

Then, provided that the iteration vectors in $\underline{X}_1$ are not orthogonal to one of the required eigenvectors (and assuming an appropriate ordering of the vectors), we have

$$\underline{\Lambda}_{k+1} \to \underline{\Lambda} \; ; \qquad \underline{X}_{k+1} \to \underline{\Phi} \quad \text{as} \quad k \to \infty \; .$$

The essential ingredients of the subspace iteration above are the simultaneous vector inverse iteration in Eq. (4) and the use of the Rayleigh minimum principle in Eqs. (5) to (8). Since inverse iteration is used, subspace iteration is closely related to the QR method [7, p. 470], but subspace iteration displays much better convergence characteristics because the Rayleigh minimum principle is employed to extract in each iteration the "best" eigenvalue and vector approximations. The use of the principle of minimizing the Rayleigh quotient of an iteration vector has also been explored by Fried [8], Falk [9], and Schwarz [3]. However, the effectiveness of subspace iteration derives from the fact that the iteration is performed with q vectors, where $q \geq p$, which are used simultaneously in the minimization of the Rayleigh quotient.

Considering the convergence of subspace iteration, two distinct features are observed, which are both important in practical analysis; namely, the minimization of the Rayleigh quotient that yields best approximations to the required eigenpairs in the current subspace and the ultimate convergence rate of the iterates. We discuss both aspects in the following sections.

3. Minimization of Rayleigh Quotient in Subspace Iteration

The Rayleigh minimum principle states that

$$\lambda_1 = \min \rho(\underline{\varphi}) \quad , \tag{9}$$

where the minimum is taken over all possible vectors $\underline{\varphi}$, and

$$\rho(\underline{\varphi}) = \frac{\underline{\varphi}^T \underline{K} \underline{\varphi}}{\underline{\varphi}^T \underline{M} \underline{\varphi}} \ . \tag{10}$$

Assuming that $\underline{K}$ and $\underline{M}$ are positive definite matrices, or that $\underline{M}$ is positive semi-definite in case $\underline{M}$ is a diagonal matrix, we have

$$0 < \lambda_1 \leq \rho(\underline{\varphi}) \leq \lambda_n \leq \infty \ . \tag{11}$$

In the k'th subspace iteration we solve for the vectors $\bar{\underline{x}}_1, \bar{\underline{x}}_2, \ldots,$ which are stored in $\bar{\underline{X}}_{k+1}$, and use the Rayleigh minimum principle as a mechanism to generate "best" eigenvalue and vector approximations. The fact that indeed the Rayleigh minimum principle is used can be demonstrated by defining a typical vector $\bar{\underline{\varphi}}$ in the subspace E_{k+1} as

$$\bar{\underline{\varphi}} = \sum_{i=1}^{q} y_i \bar{\underline{x}}_i \quad . \tag{12}$$

Then substituting $\bar{\underline{\varphi}}$ into Eq. (10) and using the conditions $\partial\rho(\bar{\underline{\varphi}})/\partial y_i = 0$, $i = 1, \ldots, q$, which must be satisfied at the minimum of $\rho(\bar{\underline{\varphi}})$, we obtain the eigenproblem

$$\bar{\underline{K}}\underline{y} = \rho \bar{\underline{M}}\underline{y} \quad , \tag{13}$$

where the elements (i, j) of $\bar{\underline{K}}$ and $\bar{\underline{M}}$ are $\bar{\underline{x}}_i^T \underline{K} \bar{\underline{x}}_j$ and $\bar{\underline{x}}_i^T \underline{M} \bar{\underline{x}}_j$, respectively. The solution to Eq. (13) can be written

$$\bar{\underline{K}}\underline{Y} = \bar{\underline{M}}\underline{Y}\underline{\rho} \quad , \tag{14}$$

where the matrix $\underline{Y}$ stores the eigenvectors of Eq. (13) and $\underline{\rho}$ is a diagonal matrix storing the corresponding eigenvalues, $\underline{\rho} = \text{diag}(\rho_i)$. The elements ρ_i are the approximations to the required eigenvalues of Eq. (1) calculated using the Rayleigh minimum principle and the corresponding eigenvector approximations are

$$\bar{\underline{\varphi}}_j = \sum_{i=1}^{q} y_{ij} \bar{\underline{x}}_i \quad ; \qquad j = 1, 2, \ldots, q \quad , \tag{15}$$

where y_{ij} is element (i, j) of $\underline{Y}$. On comparing now Eqs. (13) to (15) with Eqs. (5) to (8), it is realized that in the k'th subspace iteration the same eigenproblem as in the minimization of the Rayleigh quotient is solved; i.e., Eq. (7) and Eq. (14) are the same equations, and that also the same eigenvector approximations are calculated.

Using the fact that the Rayleigh minimum principle is employed to evaluate in each subspace iteration the new eigenvalue and vector approximations, it follows that in the k'th subspace iteration,

$$\lambda_1 \leq \lambda_1^{(k+1)} \quad ; \quad \lambda_2 \leq \lambda_2^{(k+1)} \quad ; \quad \cdots \quad ; \quad \lambda_q \leq \lambda_q^{(k+1)} \leq \lambda_n \tag{16}$$

and, in particular, it is possible to show the actual mechanism used to calculate the values $\lambda_i^{(k+1)}$. The condition that $\lambda_1 \leq \lambda_1^{(k+1)}$ follows from Eq. (9), because the subspace E_{k+1} is contained in the n-dimensional space in which $\underline{K}$ and $\underline{M}$ are defined.

The inherent procedure employed to evaluate $\lambda_2^{(k+1)}$ demonstrates the mechanism used to evaluate the approximations to the higher eigenvalues. First we observe that as an extension of the Rayleigh minimum principle, the minimax characterization of eigenvalues gives [7],

$$\lambda_2 = \min \rho(\underline{\varphi}) \ , \tag{17}$$

where the minimum is taken over all $\underline{\varphi}$ subject to the restriction

$$\underline{\varphi}^T \underline{M} \underline{\varphi}_1 = 0 \ . \tag{18}$$

However, in the subspace iteration we have using the notation of Eq. (12),

$$\bar{\underline{\varphi}}_i^T \underline{M} \bar{\underline{\varphi}}_j = \delta_{ij} \ , \tag{19}$$

where δ_{ij} is the Kronecker delta. Hence,

$$\lambda_2^{(k+1)} = \min \rho(\bar{\underline{\varphi}}) \quad , \tag{20}$$

where the minimum is taken over all possible vectors $\bar{\underline{\varphi}}$ defined in Eq. (12) that satisfy the orthogonality condition

$$\bar{\underline{\varphi}}^T \underline{M} \bar{\underline{\varphi}}_1 = 0 \quad . \tag{21}$$

To prove that $\lambda_2 \leq \lambda_2^{(k+1)}$ we consider the auxiliary problem of evaluating $\tilde{\lambda}_2^{(k+1)}$, where

$$\tilde{\lambda}_2^{(k+1)} = \min \rho(\bar{\underline{\varphi}}) \tag{22}$$

subject to the condition

$$\bar{\underline{\varphi}}^T \underline{M} \underline{\varphi}_1 = 0 \quad . \tag{23}$$

However, since $\lambda_2 \leq \tilde{\lambda}_2^{(k+1)}$, because E_{k+1} is contained in the space spanned by $\underline{\varphi}_1, \ldots, \underline{\varphi}_n$, and also $\tilde{\lambda}_2^{(k+1)} \leq \lambda_2^{(k+1)}$, because the restriction in Eq. (21) is the most severe one, we conclude that $\lambda_2 \leq \lambda_2^{(k+1)}$.

In analogy to the conclusion reached on the calculation of $\lambda_2^{(k+1)}$, we can conclude that in the subspace iteration, we evaluate

$$\lambda_i^{(k+1)} = \min \rho(\bar{\underline{\varphi}}) \tag{24}$$

subject to the constraint,

$$\bar{\underline{\varphi}}^T \underline{M} \bar{\underline{\varphi}}_j = 0 \quad , \qquad j = 1, \ldots, i-1 \quad . \tag{25}$$

Hence, in the calculation of the approximation to the i'th eigenpair, (i-1) constraint equations have to be satisfied. This observation indicates that in the subspace iteration the higher eigenvalues and corresponding eigenvectors are, in general, calculated with less accuracy than the lower eigenpairs, for which less constraints are imposed. This fact is also observed in practical eigensolutions.

Another important deduction can also be made from the above results, namely that the required eigenvalues and eigenvectors are calculated immediately if E_{k+1} contains the subspace corresponding to $\underline{\varphi}_1, \ldots, \underline{\varphi}_p$. In other words, if linear combinations of the vectors in $\bar{\underline{X}}_{k+1}$ can yield the required eigenvectors, then these eigenvectors are calculated using Eqs. (5) to (8).

4. Convergence Analysis

In the previous section we discussed the mechanism that is used to establish optimum approximations to the required eigenvalues and eigenvectors in a specific subspace, and we also deduced that if the subspace converged, the eigenvalues and vectors calculated are those required. However, we did not discuss the convergence of the vector iterates to the required subspace and the ultimate rate of convergence.

Following the work of Rutishauser [10], the convergence of the subspace iterations is conveniently studied by first changing basis from the finite element coordinate basis to the basis of eigenvectors [7, p. 425]. This change of basis is achieved using the following relation for the vectors $\underline{X}_k$ in Eq. (4),

$$\underline{X}_k = \underline{\Phi}\underline{Z}_k \quad , \tag{26}$$

where $\underline{\Phi}$ is the matrix storing all eigenvectors, $\underline{\Phi} = [\underline{\varphi}_1, \ldots, \underline{\varphi}_n]$. Since $\underline{\Phi}$ is nonsingular, there is a unique $\underline{Z}_k$ for any $\underline{X}_k$, and vice versa.

Introducing the relation of Eq. (26) into Eq. (4) and premultiplying by $\underline{\Phi}^T$ we obtain for the first equation that is solved in subspace iteration,

$$\underline{\Lambda}\underline{\bar{Z}}_{k+1} = \underline{Z}_k \tag{27}$$

and then equations equivalent to Eqs. (5) to (8), but which express the relations in the new basis, are used to evaluate $\underline{Z}_{k+1}$. The convergence rate of the iteration is established from Eq. (27) and using the fact that in the subspace iterations always the optimum approximations to the required eigenvalues and eigenvectors are calculated.

For the convergence analysis let the iteration matrix $\underline{Z}_k$ be denoted as follows,

$$\underline{Z}_k = \begin{bmatrix} 1 & 0 & \cdots & 0 \\ 0 & 1 & & 0 \\ 0 & 0 & & \cdot \\ 0 & 0 & & \cdot \\ \vdots & \vdots & & 0 \\ 0 & 0 & & 1 \\ z_{q+1,1}^{(k)} & z_{q+1,2}^{(k)} & \cdots & z_{q+1,q}^{(k)} \\ z_{q+2,1}^{(k)} & z_{q+2,2}^{(k)} & \cdots & z_{q+2,q}^{(k)} \\ \vdots & \vdots & & \\ z_{n,1}^{(k)} & z_{n,2}^{(k)} & \cdots & z_{n,q}^{(k)} \end{bmatrix}, \tag{28}$$

where $\underline{Z}_k$ is completely general, because the unit $q \times q$ matrix $\underline{I}$ can always be obtained by linearly combining columns, provided $\underline{Z}_k$ is not deficient in the vectors $\underline{e}_i$, $i = 1, \ldots, q$. Using Eq. (27) we then obtain,

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$$\bar{\underline{Z}}_{k+1} = \begin{bmatrix} 1/\lambda_1 & 0 & & 0 \\ 0 & 1/\lambda_2 & & \cdot \\ 0 & 0 & & \cdot \\ \vdots & \vdots & & 0 \\ 0 & 0 & & 1/\lambda_q \\ z^{(k)}_{q+1,1}/\lambda_{q+1} & z^{(k)}_{q+1,2}/\lambda_{q+1} & \cdots & z^{(k)}_{q+1,q}/\lambda_{q+1} \\ z^{(k)}_{q+2,1}/\lambda_{q+2} & z^{(k)}_{q+2,2}/\lambda_{q+2} & \cdots & z^{(k)}_{q+2,q}/\lambda_{q+2} \\ \vdots & \vdots & & \vdots \\ z^{(k)}_{n,1}/\lambda_n & z^{(k)}_{n,2}/\lambda_n & \cdots & z^{(k)}_{n,q}/\lambda_n \end{bmatrix} . \tag{29}$$

The subspace E_{k+1} spanned by $\bar{\underline{Z}}_{k+1}$ is not changed if we multiply column i in $\bar{\underline{Z}}_{k+1}$ by λ_i, i.e., E_{k+1} is also spanned by $\tilde{\underline{Z}}_{k+1}$, where

$$\tilde{\underline{Z}}_{k+1} = \begin{bmatrix} 1 & 0 & & 0 \\ 0 & 1 & & \cdot \\ \cdot & 0 & & \cdot \\ \cdot & \vdots & & 0 \\ 0 & 0 & & 1 \\ z^{(k)}_{q+1,1}\dfrac{\lambda_1}{\lambda_{q+1}} & z^{(k)}_{q+1,2}\dfrac{\lambda_2}{\lambda_{q+1}} & \cdots & z^{(k)}_{q+1,q}\dfrac{\lambda_q}{\lambda_{q+1}} \\ z^{(k)}_{q+2,1}\dfrac{\lambda_1}{\lambda_{q+2}} & z^{(k)}_{q+2,2}\dfrac{\lambda_2}{\lambda_{q+2}} & \cdots & z^{(k)}_{q+2,q}\dfrac{\lambda_q}{\lambda_{q+2}} \\ \vdots & \vdots & & \vdots \\ z^{(k)}_{n,1}\dfrac{\lambda_1}{\lambda_n} & z^{(k)}_{n,2}\dfrac{\lambda_2}{\lambda_n} & & z^{(k)}_{n,q}\dfrac{\lambda_q}{\lambda_n} \end{bmatrix} . \tag{30}$$

But in the previous section we have shown that in Eqs. (5) to (8) we calculate the best approximations to the eigenvectors that can be extracted from $\bar{\underline{X}}_{k+1}$. Similarly, in the subspace iteration using Eq. (27) the best eigenvector approximations are extracted from the vectors stored in $\bar{\underline{Z}}_{k+1}$. But on inspecting the columns of $\tilde{\underline{Z}}_{k+1}$ in Eq. (30) we find that ultimately the i'th column is the best approximation to the vector $\underline{e}_i$ in the subspace E_{k+1}. The order and ultimate rate of convergence to the i'th eigenvector is thus obtained by evaluating

$$\frac{\| \tilde{\underline{z}}_i^{(k+1)} - \underline{e}_i \|_2}{\| \underline{z}_i^{(k)} - \underline{e}_i \|_2} = \frac{\lambda_i}{\lambda_{q+1}} \sqrt{\frac{\sum_{j=1}^{n-q} \left(z_{q+j,i}^{(k)} \right)^2 \left(\frac{\lambda_{q+1}}{\lambda_{q+j}} \right)^2}{\sum_{j=1}^{n-q} \left(z_{q+j,i}^{(k)} \right)^2}} , \qquad (31)$$

where $\underline{z}_i^{(k)}$ is the i'th column of $\underline{Z}_k$, and similar for $\tilde{\underline{z}}^{(k+1)}$. Hence,

$$\frac{\| \tilde{\underline{z}}_i^{(k+1)} - \underline{e}_i \|_2}{\| \underline{z}_i^{(k)} - \underline{e}_i \|_2} \le \frac{\lambda_i}{\lambda_{q+1}} \qquad (32)$$

and convergence is linear with the rate of convergence equal to λ_i/λ_{q+1}. We, therefore, conclude that provided the columns in $\underline{X}_{k+1}$ in Eqs. (4) and (8) are ordered appropriately, and provided the starting subspace is not orthogonal to the required least dominant subspace spanned by $\underline{\varphi}_1, \ldots, \underline{\varphi}_q$, the i'th column in $\underline{X}_{k+1}$ converges linearly with the rate λ_i/λ_{q+1} to $\underline{\varphi}_i$. Since the eigenvalues are calculated using the Rayleigh quotient, the i'th eigenvalue in Eq. (7) converges linearly with the rate $(\lambda_i/\lambda_{q+1})^2$ to λ_i.

5. Selection of Starting Subspace

The first step in the subspace iteration method is the selection of the starting iteration vectors in $\underline{X}_1$. We showed that if starting iteration vectors are used that span the least dominant p-dimensional subspace of $\underline{K}$ and $\underline{M}$, the subspace iteration in Eqs. (4) to (8) calculates in the first iteration the required vectors $\underline{\varphi}_1, \ldots, \underline{\varphi}_p$. The aim in the selection of the starting iteration vectors is, therefore, to obtain vectors that as closely as possible span the least dominant subspace of $\underline{K}$ and $\underline{M}$.

Two cases for which the starting vectors can be chosen to span exactly the least dominant subspace of $\underline{K}$ and $\underline{M}$ are, firstly, when the mass matrix is a diagonal matrix with only q nonzero masses and, secondly, when $\underline{K}$ and $\underline{M}$ are both diagonal matrices.

In the case of a diagonal mass matrix with only q nonzero diagonal mass elements, the first subspace iteration yields

$$\begin{bmatrix} \underline{K}_{aa} & \underline{K}_{ac} \\ \underline{K}_{ca} & \underline{K}_{cc} \end{bmatrix} \underline{\bar{X}}_2 = \begin{bmatrix} \underline{M} & \underline{0} \\ \underline{0} & \underline{0} \end{bmatrix} \begin{bmatrix} \underline{I} \\ \underline{0} \end{bmatrix} , \qquad (33)$$

where

$$\underline{\bar{X}}_2 = \begin{bmatrix} \underline{\bar{F}}_a \\ \underline{\bar{F}}_c \end{bmatrix} . \qquad (34)$$

The projections of $\underline{K}$ and $\underline{M}$ are

$$\underline{K}_2 = \underline{\bar{F}}_a^T \underline{M} \qquad (35)$$

and

$$\underline{M}_2 = \underline{\bar{F}}_a^T \underline{M} \underline{\bar{F}}_a \quad . \qquad (36)$$

The eigenproblem corresponding to the projected matrices is thus

$$\bar{F}_a^T M x = \lambda \bar{F}_a^T M \bar{F}_a x \quad . \tag{37}$$

Now substituting $\bar{F}_a = F_a M$, where $F_a^{-1} = K_a$ and K_a is the stiffness matrix obtained by statically condensing out in K all zero mass degrees of freedom, we realize that Eq. (37) can be rewritten as

$$K_a x = \lambda M x \quad . \tag{38}$$

But Eq. (38) is the eigenproblem from which all finite eigenvalues of Eq. (1) are evaluated. Hence, we obtain in the first subspace iteration the lowest q finite eigenvalues and corresponding eigenvectors.

In the second case, when K and M are both diagonal matrices, which is really a trivial case, the unit entries in the unit starting iteration vectors are chosen to correspond to the smallest values of k_{ii}/m_{ii}. Thus, the unit starting vectors are already multiples of the required eigenvectors and the values k_{ii}/m_{ii} are the corresponding required eigenvalues.

In practice, the specific matrices assumed above are hardly encountered, but the results concerning the construction of the starting iteration vectors indicate, how in general analysis effective starting vectors can be established. The fundamental observation is that in both cases above the degrees of freedom with the smallest ratios k_{ii}/m_{ii} are excited, and because the mass of the system was already lumped to a sufficient extent, convergence is obtained in one subspace iteration. If mass is not lumped to the extent used in the two cases above, iteration is required, but the starting vectors should still be unit vectors with their entries corresponding to the degrees of freedom with the smallest values k_{ii}/m_{ii}. The actual scheme proposed in [4], which has been employed extensively, uses as the first column in MX_1 the diagonal of the mass matrix M, and as the next columns unit vectors with their entries +1 corresponding to the smallest ratios k_{ii}/m_{ii}. The first full column is used in order to excite all mass degrees of freedom. Since we are iterating with q vectors, $q \geq p$, when we want to converge to p vectors, the $(q-1)$ unit vectors would assure convergence in one subspace iteration if one of the two special cases above is considered.

It has been claimed that starting iteration vectors with random numbers are sufficiently effective [10, 11]. Based on the above observations, and some numerical experiments, it is believed that in most cases the above starting subspace is considerably more effective than the use of random numbers in the starting vectors. But to improve the solution characteristics it is recommended that the q'th iteration vector be a random vector and be generated new in each iteration.

In addition to considering the degrees of freedom corresponding to the smallest values k_{ii}/m_{ii}, it appears that an additional important consideration can be derived from the values $k_{ij}^2/(k_{ii}k_{jj})$. Physically, the magnitude of the value $k_{ij}^2/(k_{ii}k_{jj})$ is a measure of the coupling between the degrees of freedom i and j. However, if this coupling is high, it is probably not effective to excite both degrees of freedom i and j in the starting iteration vectors, because "stiff" relative displacements are only activated in the higher modes.

6. Acceleration of Convergence

In the solution of some problems, notably those with high mass lumping, only a few subspace iterations, say 6 to 8, are required for convergence to 6 digit precision on the eigenvalues. However, when systems with a continuous mass distribution are considered, such as dams, a large number of iterations may be required. In such cases, schemes to accelerate the convergence are very desirable.

6.1 Shifting

One way to accelerate convergence is to impose a shift μ onto the matrix $\underset{\sim}{K}$, i.e., to iterate on the matrix $\underset{\sim}{K} - \mu \underset{\sim}{M}$ rather than on $\underset{\sim}{K}$. In order to preserve stability and convergence to the required lowest eigenvalues and eigenvectors it is necessary to choose the shift judiciously. A conservative value for μ is $\mu < \lambda_1$, and in practice we may choose $\mu = 0.9\lambda_1$. However, it then follows that μ can only be chosen once λ_1 has been approximated to a sufficient accuracy (say, to three digits), which means that the shift will be imposed after the first few subspace iterations. The new rate of convergence of the i'th iteration vector to the i'th eigenvector is then $(\lambda_i - \mu)/(\lambda_{q+1} - \mu)$. It is noted that this shifting will, therefore, greatly increase the rate of convergence to the lower eigenvalues, but if q is large the rate of convergence to the higher eigenvalues of the required spectrum may only be marginally increased.

Together with imposing a shift Chebyshev polynomials may also be employed in the iteration vectors to accelerate the convergence [10][12]. Although some experience has been obtained, the overall effectiveness of using Chebyshev polynomials in the eigensolution of large systems has not been established as yet.

For small banded systems, the determinant search algorithm presented in [7] has proven to be efficient, and it appears that depending on the bandwidth of the system the shifting strategies used in that technique could be very effective in subspace iterations.

6.2 Use of Aitken's acceleration process

Assume that we have calculated $\underset{\sim}{X}_k, \underset{\sim}{X}_{k+1}, \underset{\sim}{X}_{k+2}$, then using Aitken's acceleration technique, improved iteration vectors for $\underset{\sim}{X}_{k+2}$ are obtained by calculating [13]

$$x_{ij}^{(k+2)} \longleftarrow x_{ij}^{(k)} - \left(x_{ij}^{(k)} - x_{ij}^{(k+1)}\right)^2 \Big/ \left(x_{ij}^{(k)} - 2x_{ij}^{(k+1)} + x_{ij}^{(k+2)}\right) \quad , \quad (39)$$

where $x_{ij}^{(k)}$ is element (i, j) of $\underline{X}_k$. Aitken's acceleration procedure has been applied successfully in iteration methods and the use of the technique in subspace iteration might, therefore, be promising.

A practical disadvantage using Aitken's acceleration technique may already be noted. Namely, not only the current iteration vectors, but also the vectors from the two preceding iterations must be stored in high speed storage or on back-up storage, because they are used whenever the improved iteration vectors are calculated as given in Eq. (39).

6.3 Overrelaxation

It is an established fact that overrelaxation can reduce the number of iterations required in the solution of systems of linear equations [7][14]. Specifically, in the Gauss-Seidel method with successive overrelaxation, the number of iterations required for convergence can be reduced by a factor of 2 or more. Similar improvements have been observed in the iterative solution of eigenproblems, when searching for the minimum of the Rayleigh quotient [3]. It appears, therefore, that in some cases overrelaxation might also significantly improve the convergence characteristics of the subspace iteration method.

To incorporate overrelaxation into the subspace iterations, Eqs. (4) to (7) remain unaltered, but the new iteration vectors $\underline{X}_{k+1}$ are obtained from

$$\underline{X}_{k+1} = \underline{X}_k + \omega(\bar{\underline{X}}_{k+1}\underline{Q}_{k+1} - \underline{X}_k) \quad , \qquad (40)$$

where ω is the overrelaxation factor.

For an analysis of the effect of the overrelaxation factor, we consider the eigenproblem formulated in the basis of the eigenvectors. The convergence analysis in Section 4 shows that we would like to have

$$\tilde{\underline{Z}}_{k+1} \rightarrow \begin{bmatrix} \underline{I} \\ \underline{0} \end{bmatrix} \; . \qquad (41)$$

But then using Eq. (40) we conclude that ω should be selected such that

$$z_{q+i,j} + \omega\left(z_{q+i,j}\,\frac{\lambda_j}{\lambda_{q+i}} - z_{q+i,j}\right) = 0 \;, \qquad \begin{array}{l} i = 1,\ldots,n-q \\ j = 1,\ldots,q \;. \end{array} \qquad (42)$$

which gives

$$\omega = \frac{1}{1 - \lambda_j/\lambda_{q+i}} \; . \qquad (43)$$

Hence, it appears that a different ω should be employed for each iteration vector $j = 1,\ldots,q$. Although we could, based on the current eigenvalue approximations, at best estimate appropriate ω-values for the iteration vectors, Eq. (43) shows that ω should be larger than one.

7. Some Numerical Solutions

To study in a preliminary manner the convergence characteristics of the subspace iteration method with and without the acceleration schemes discussed above, the solution of a few eigenproblems was considered. The immediate aim was to identify whether the acceleration schemes would indeed be reducing the number of iterations considerably. The next step of this work will be to optimize the acceleration schemes and develop an improved subspace iteration method.

Figure 1 summarizes the discrete systems that have been analyzed in this study using the subspace iteration method, and gives the size and order of the corresponding stiffness and mass matrices.

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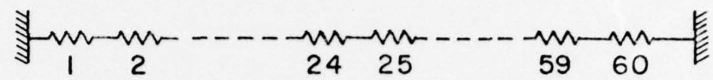
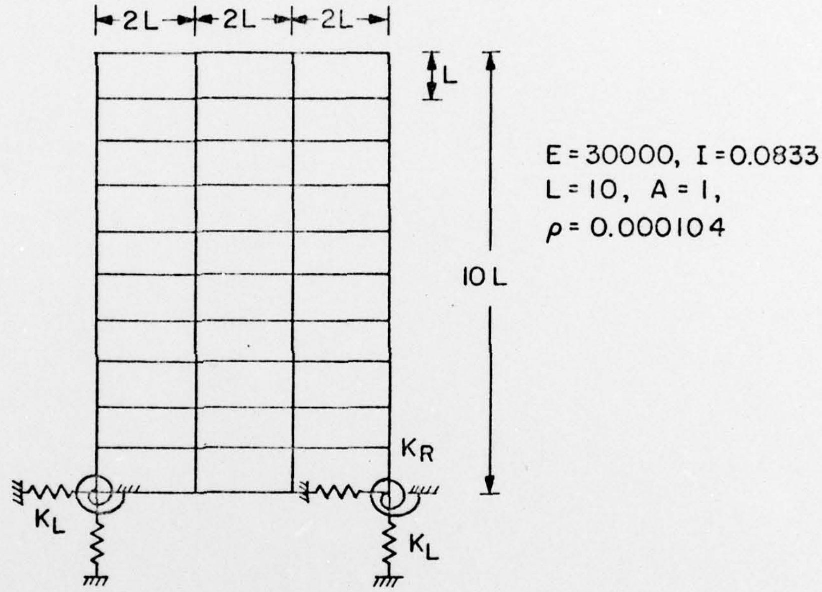


EXAMPLE 1 ANALYSIS OF 60 ELEMENT UNIFORM SPRING MODEL



EXAMPLE 2 ANALYSIS OF 10 STOREY AND 3 BAY FRAME ON SPRING SUPPORTS

Figure 1. Sample analyses.

These problems have been selected because a relatively large number of iterations are required for solution of the required eigenpairs.

Tables 2 and 3 summarize the results obtained in the analyses. Convergence in the iterations was measured by [7, p. 504]

Table 2. Analysis of Spring Model: k = 375; m = 0.00013; consistent mass, tol = 10^{-8}

Case	no acceleration	with over-relaxation	with shifting to μ (Sect. 6.1)	with Aitken's acceleration
number of eigenpairs	2 8 22	22	2 22	22
number of iteration vectors	4 16 30	30	4 30	30
number of iterations	7 10 25	20	6 25	26

Table 3. Analysis of Frame Model: $k_L = 10^5$; $k_R = 10^6$; lumped mass, tol = 10^{-7}

Case	no acceleration	with over-relaxation	with shifting to μ (Sect. 6.1)	with Aitken's acceleration
number of eigenpairs	2 8 22	2 8 22	2 22	2
number of iteration vectors	4 16 30	4 16 30	4 30	4
number of iterations	25 14 18	16 12 20	11 18	25

$$\frac{|\lambda_i^{(k+1)} - \lambda_i^{(k)}|}{\lambda_i^{(k+1)}} \leq \text{tol} \quad , \qquad i = 1,\ldots,p \ ,$$

where $\lambda_i^{(k)}$ is the approximation to λ_i calculated in the k'th subspace iteration. The results in the tables display the following solution features.

Using the overrelaxation scheme with an arbitrarily picked value $\omega = 1.6$ for all iteration vectors the number of iterations required for convergence was reduced in almost all cases.

Considering shifting to a lower bound on λ_1, it is seen that the number of iterations required for convergence is reduced significantly when only a small number of eigenpairs are sought but, as expected, when relatively many eigenpairs are to be extracted a single shift into the vicinity of the smallest eigenvalue required does not result in a substantial decrease in the total number of subspace iterations needed.

Since shifting accelerates the convergence to the eigenvalues in the vicinity of the shift, additional shifting to the higher eigenvalues should be performed, but a stable and effective algorithm is still to be developed.

In these analyses the Aitken acceleration did not reduce the total number of subspace iterations required for solution. In addition, it was observed that the process of using Aitken's acceleration was very sensitive to the time at which the acceleration was applied. It was found that Aitken's formula should only be employed once the iteration vectors converged linearly, otherwise the application of the formula could result in an increase of the number of iterations needed for the solution.

8. Conclusions

Based on the theoretical convergence study of subspace iteration and the few numerical experiments presented in this paper, it is concluded that the original subspace iteration method can, for many eigensolutions, still be improved significantly. Improvements in the starting subspace should be possible. Among the acceleration techniques presented in the paper the use of overrelaxation factors appears very promising. In addition, shifting strategies as employed in the determinant search method should be explored.

In this paper, the use of the subspace iteration method was only considered for the calculation of the smallest eigenvalues and corresponding eigenvectors but the development of shifting strategies should also lead to an extension of the technique to be able to calculate intermediate eigenvalues.

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Chapter 20

NUMERICAL CONTINU
APPLICATIONS

Werner C. Rheinboldt

1. Introduction

Finite dimensional anal
problems usually assur
equation

Fx = 0

with a given mapping

$F: D \subset R^n \to R^n,\ x = (x_1$

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and approximations.
applications the follow

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of the variables
(b) The computatio
its derivative F
(c) In general, the

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