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Iterative procedures related to relaxation methods for eigenvalue problems

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Three iterative procedures for approximating to the solutions of linear eigenvalue problems for systems with a finite number of degrees of freedom are discussed. Two of the procedures are closely related to known iterative procedures while the third is original. The procedures are shown to possess quadratic, geometric and cubic convergence. All three procedures lie within the framework of the relaxation method, each representing a particular manner of fixing the freedom of choice existent in the relaxation method. The study was made to investigate the convergence and behaviour in the large of the relaxation method and to provide guiding principles for the relaxation computer. One particular result of importance is that orthogonalization of trial modes is not essential to the success of the relaxation method.

The relaxation method developed by Southwell and others (Southwell 1940; Allen, Fox, Motz & Southwell 1941) provides a powerful approximate procedure for the solution of eigenvalue problems in systems with a finite number of degrees of freedom. A theoretical investigation of the procedure was recently made by Cooper (1948), who showed the convergence of the method for the extreme eigenvalues. For the intermediate eigenvalues, both Southwell, in his examples, and Cooper,* in his discussion, proceed by orthogonalizing the new trial modes with respect to those already determined. The present investigation has two objectives: first, to show that orthogonalization is not essential to the success of the method; and secondly, to investigate the overall behaviour of the process in order to provide guiding principles for the computer.

A unique feature of relaxation methods is that they are approximate procedures which are not rigidly prescribed in advance. The precise procedure to be followed is not dictated but is left to the intuition and accumulated experience of the computer. The computer's intelligence is thus an active or dynamic link in the computational chain. It is this fact which has made relaxation so attractive to many computers. The concept of convergence for such a flexible process is, however, somewhat lacking in precision. I propose to call a relaxation procedure convergent if within its framework a convergent iterative procedure can be constructed by inserting initially fixed criteria into all steps requiring judgement on the part of the computer. For eigenvalue problems three distinct convergent iterative procedures will be shown all related to the relaxation method which exhibit, respectively, quadratic convergence, geometric convergence and cubic convergence. (An iterative procedure, with error ϵ after k steps, is said to have (a) geometric, (b) quadratic, (c) cubic convergence, if after $k+1$ steps the error is of order (a) $\delta\epsilon$, (b) ϵ^2 , (c) ϵ^3 , where δ is a constant, independent of k , satisfying $0 < \delta < 1$). The behaviour in the large of the three methods is also

* The orthogonalization device used by Cooper is called deflation by Aitken (1937).

investigated. It is not suggested that any of the iterative procedures would be more useful to the computer than the original relaxation method, but rather it is hoped that a knowledge of the behaviour of these related methods will enable the computer to make more efficient use of the freedom of relaxation.

1. DESCRIPTION OF THE PROBLEM

We take the linear eigenvalue problem in the following form which includes both lumped parameter systems and the finite difference analogues of continuous systems. Let A and B be given real symmetric matrices of order n with elements a_{ij} and b_{ij} , and, moreover, let the b_{ij} be the coefficients of a positive definite quadratic form. Then the eigenvectors or modes $X(x_1, x_2, \dots, x_n)$ and eigenvalues λ are to be determined from the equation

$$AX = \lambda BX. \tag{1}$$

It is known that there are n eigenvalues $\lambda_i (i = 1, 2, \dots, n)$ and n corresponding modes $X_i (i = 1, 2, \dots, n)$ which we will take to be orthonormal with respect to B ; i.e.

$$X_i BX_j = \begin{cases} 0, & i \neq j \\ 1, & i = j \end{cases}. \tag{2}$$

We also know that any vector $V(v_1, v_2, \dots, v_n)$ may be expanded uniquely in terms of these eigenvectors in either of the following ways:

$$V = \sum_{i=1}^n c_i X_i = \sum_{i=1}^n d_i BX_i.$$

In the relaxation method for solving (1) residual vectors $R(r_1, r_2, \dots, r_n)$ are associated with trial vectors V and trial eigenvalues Λ as follows:

$$R = AV - \Lambda BV. \tag{3}$$

Starting from an initial trial vector, V , the first trial Λ is obtained by forming Rayleigh's quotient for V , i.e.

$$\Lambda = \frac{V'AV}{V'BV},$$

where V' is the transpose of V . Now with this value of Λ fixed in (3), the vector V is altered with intent to reduce the residual vector R . This operation is facilitated by the use of relaxation operations tables. The amount of alteration in V and R is not specified, but when, in the opinion of the computer, the residual has been 'sufficiently reduced', Rayleigh's quotient is re-computed for the altered V and the process repeated as many times as the computer deems necessary. In a large number of examples, engineering accuracy has been obtained with no more than two or three recomputations of Λ . In these cases the computer was experienced and had some intuitional basis for choosing the initial trial V .

In the iterative procedures which follow we shall consider equation (3) to define the vector V for prescribed R and Λ . We note here that if Λ is not an eigenvalue, λ , of (1), then there is a unique V for every R . In fact, if in (3) the residual is expanded in the form

$$R = \sum_{i=1}^n h_i BX_i, \tag{4}$$

and we assume for V the expression

$$V = \sum_{i=1}^n c_i X_i, \quad (5)$$

it is possible to evaluate the c_i by premultiplying (3) with X'_i , and by using (1) and (2) to get

$$V = \sum_{i=1}^n \frac{h_i}{\lambda_i - \Lambda} X_i. \quad (6)$$

However, if $\Lambda = \lambda_p$, then there exist two possibilities. If in the expansion (4) $h_p \neq 0$, then there exists no finite solution to (3). On the other hand, if h_p (and all h_i associated with λ_p if λ_p is a multiple root)* vanishes, then a multiplicity of solutions exist. Thus if we consider V to be expanded as in (5), the c_i ($i \neq p$) would be uniquely determined, but c_p would be arbitrary. In attempting to find V from (3), the occurrence of the first-named possibility would indicate that Λ was an eigenvalue and hence the corresponding mode could be determined. We will assume that in the second case the multiplicity of solutions would not be noticed and hence the fact that Λ was an eigenvalue would not be discovered.

2. AN ITERATIVE PROCEDURE WITH QUADRATIC CONVERGENCE

The following method is a slight extension of one suggested by Rayleigh (1945) and recently re-suggested by Kohn (1949). We choose a fixed residual vector, R , and then use equation (3) to obtain vectors V corresponding to scalars Λ . The Λ are in turn obtained as the Rayleigh quotients of the preceding vectors V . The Rayleigh-Kohn† method is the special case where the residual R (r_1, r_2, \dots, r_n) has the form: $r_i = 0$, $i \neq p$ and $r_p = 1$. In general, let the fixed residual R have the expansion (4). The process may be started with a choice of an initial vector V_0 , or of an initial scalar Λ_1 . The succeeding steps are described by the following recursion formulae:

$$\Lambda_{k+1} = \frac{V'_k A V_k}{V'_k B V_k} \quad (k = 0, 1, 2, \dots), \quad (7)$$

$$R = (A - \Lambda_{k+1} B) V_{k+1} \quad (k = 0, 1, 2, \dots). \quad (8)$$

The scalars Λ_k are obtained from (7) and the vectors V_k are determined by (8). With the aid of (6) it is possible to give the more explicit forms of V_k and Λ_{k+1} :

$$V_k = \sum_{i=1}^n \frac{h_i}{\lambda_i - \Lambda_k} X_i, \quad (9)$$

$$\Lambda_{k+1} = \frac{\sum_{i=1}^n \frac{h_i^2 \lambda_i}{(\lambda_i - \Lambda_k)^2}}{\sum_{i=1}^n \frac{h_i^2}{(\lambda_i - \Lambda_k)^2}}. \quad (10)$$

The quadratic convergence of the process can be seen from (10). If $\Lambda_k = \lambda_p + \epsilon$, where $|\epsilon|$ is small compared with the eigenvalue spacing, then it follows that if h_p is non-zero, we have

$$\Lambda_{k+1} = \lambda_p + O(\epsilon^2).$$

* In what follows we assume the λ_i to be distinct. Obvious modifications in the statements would be required for multiple roots.

† It may be noted that the tabular procedure of Holzer for torsional vibration (see Den Hartog 1947) and also Mykelstad's (1944) tabular procedure for flexural vibrations are both of this type as regards computation of the vector V . However, it is not usual in these procedures to take the succeeding Λ as the Rayleigh quotient of the preceding V . Usually the succeeding Λ is chosen by intuition and the general principles of interpolation.

The behaviour of the process in the large (i.e. when Λ_k is not in the immediate neighbourhood of an eigenvalue) is fairly complicated. Considerable insight may be obtained by studying the function

$$f(\Lambda_k) = \Lambda_{k+1} - \Lambda_k = \frac{\sum_{i=1}^n \frac{h_i^2}{\lambda_i - \Lambda_k}}{\sum_{i=1}^n \frac{h_i^2}{(\lambda_i - \Lambda_k)^2}}. \tag{11}$$

A sketch of this function is shown in figure 1. An elementary analysis reveals that if m of the h_i are non-zero, then $f(\Lambda_k)$ has $(2m - 1)$ zeros; the m eigenvalues, λ_i , corresponding to the non-zero h_i , and $(m - 1)$ values, μ_i , separating these λ_i . It is readily found that the slope of $f(\Lambda_k)$ is -1 at each of these λ_i , and $+1$ at each of the μ_i .

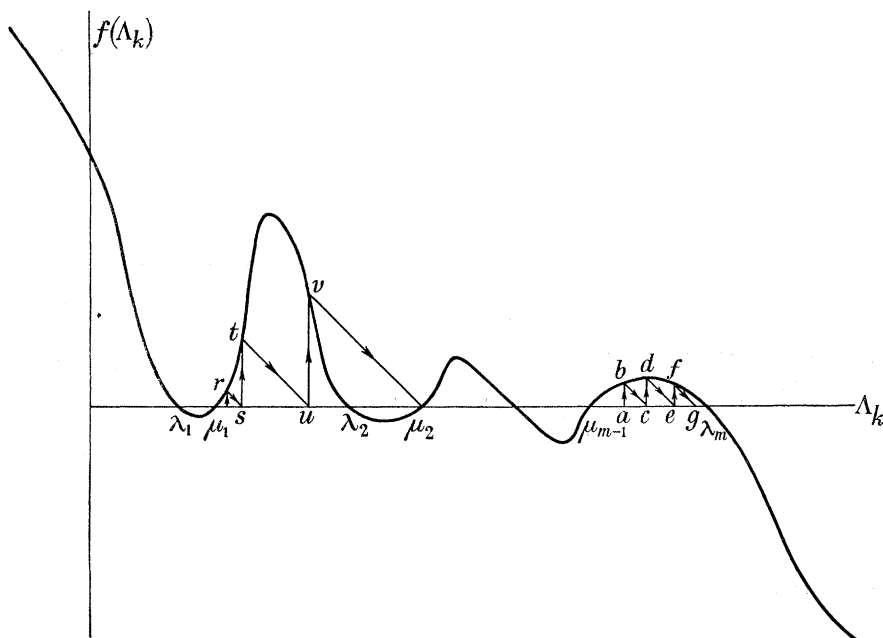


FIGURE 1

A possible iterative sequence of Λ_k converging on λ_m is indicated in the figure by the path *abcdefg*. It will be noted that the quadratic convergence in the neighbourhood of the λ_i is clearly indicated by the fact that $f(\Lambda_k)$ has slope -1 at each eigenvalue. The fact that $f(\Lambda_k)$ has slope $+1$ at each of the μ_i indicates that the μ_i are unstable foci of the process, i.e. if $\Lambda_k = \mu_p + \epsilon$, then $\Lambda_{k+1} \approx \mu_p + 2\epsilon$. However, it is possible to have a sequence of Λ_k which converge to a μ_i as is shown by the path *rstuv* μ_2 in figure 1. A little further study leads us to the following general conclusion. Starting from any initial Λ_1 , the iterative procedure described in this section yields a sequence, Λ_k ($k = 1, 2, \dots$), which does one of the following:

- (1) Sequence terminates after a finite number of steps with Λ_k equal to an eigenvalue.
- (2) Sequence terminates after a finite number of steps with Λ_k equal to an unstable focus μ_i .
- (3) After a finite number of steps, sequence becomes monotonic, approaching an eigenvalue with quadratic convergence.

The first two possibilities above have zero probability. By tracing paths such as $rstuv\mu_2$ in reverse, it is clear that the set of values of Λ_1 for which these cases can occur is denumerable. In general, then, we have the third possibility. To show that the sequence becomes monotonic we fix our attention on (10) which states that Λ_{k+1} is a weighted average of the λ_i and note that if $\Lambda_{k+1} > \Lambda_k$, the weights will be so altered as to make $\Lambda_{k+2} > \Lambda_{k+1}$ unless there are eigenvalues $\lambda_p, \lambda_{p+1}, \dots, \lambda_{p+r}$, with non-zero h_i located between Λ_k and Λ_{k+1} . In this latter case we can argue that no future Λ_k of the sequence will ever be less than λ_p , which is sufficient to assure that eventually two succeeding Λ cannot be separated by an eigenvalue.

The following general remarks may be made in connexion with this procedure:

(1) There is a neighbourhood about each eigenvalue λ_p (for which the corresponding h_p is non-zero) such that if Λ_1 is taken in this neighbourhood, the iterative procedure described in this section will converge to λ_p and to the corresponding mode X_p . The size of the neighbourhood depends on the eigenvalue spacing and the relative magnitude of h_p compared with the other h_i .

(2) For those eigenvalues, λ_q , for which $h_q = 0$ in the expansion of R , we note that there is no tendency toward convergence. If, by chance, $\Lambda_k = \lambda_q$, this fact might easily not be recognized. See the remarks at the end of § 1.

(3) The unstable foci, μ_i , can be distinguished from the eigenvalues, λ_p , by noting that for $\Lambda_k = \mu_i$ the corresponding vector V_k is uniquely determined, while for $\Lambda_k = \lambda_p$ there is no finite solution for V_k .

We next examine two related procedures which exhibit somewhat simpler behaviour in the large.

3. AN ITERATIVE PROCEDURE WITH GEOMETRIC CONVERGENCE

In the method of the previous section we fixed the residual vector R and constructed a sequence of Λ_k and V_k , using (3) together with Rayleigh's quotient. We now turn to a procedure in which Λ is fixed and a sequence of residuals, R_k , and vectors, V_k , is constructed from (3).

Having fixed Λ , we start with a trial vector V_0 . The succeeding steps are described by the following recursion formulae:

$$R_{k+1} = BV_k \quad (k = 0, 1, 2, \dots), \quad (12)$$

$$R_{k+1} = (A - \Lambda B)V_{k+1} \quad (k = 0, 1, 2, \dots). \quad (13)$$

The residuals, R_k , are determined by (12) and the vectors, V_k , are in turn obtained from (13).

If the original trial vector, V_0 , is expanded as in (5), and we use (12) and (13) k times falling back on (6) to solve (13) each time, it is possible to give the following explicit form for V_k :

$$V_k = \sum_{i=1}^n \frac{c_i}{(\lambda_i - \Lambda)^k} X_i. \quad (14)$$

The characteristics of this procedure are clearly illuminated by (14). If

$$|(\lambda_p - \Lambda)/(\lambda_i - \Lambda)| \leq \delta < 1 \quad (i \neq p \text{ and } c_p \neq 0),$$

then we can write

$$V_k = \frac{c_p}{(\lambda_p - \Lambda)^k} \left\{ X_p + \sum'_{i=1}^n \left(\frac{c_i}{c_p} \right) \left(\frac{\lambda_p - \Lambda}{\lambda_i - \Lambda} \right)^k X_i \right\}, \tag{15}$$

where the accent on the summation indicates that $i = p$ is omitted. We see that as k gets large, V_k approaches a multiple of the mode, X_p . The convergence is geometric, i.e. like terms of the geometric progression $\delta, \delta^2, \delta^3, \dots$. The rapidity of convergence depends essentially on how near Λ is taken to λ_p . The method produces an approximation for the eigenvector, X_p , but no information is given directly about the eigenvalue. An auxiliary computation would be necessary.

If Λ is taken so that $\Lambda - \lambda_p = \lambda_q - \Lambda$, and in the expansion of $V_0, c_p \neq 0, c_q \neq 0$, and, moreover, there are no other eigenvalues, λ_i with $c_i \neq 0$ between λ_p and λ_q , then the method does not converge to an eigenvector but eventually oscillates between multiples of $X_p + X_q$ and $X_p - X_q$. Considering the n eigenvalues in pairs, there are $\frac{1}{2}(n-1)n$ values of Λ for which with suitable V_0 this oscillatory behaviour is possible. If Λ is taken close to an eigenvalue, λ_p , for which $c_p = 0$, there will be no tendency to converge toward X_p . However, if Λ is taken exactly equal to λ_p , although $c_p = 0$ in the expansion of V_0 , the expansion of V_1 will in all probability contain a component of X_p , and the fact that Λ was an eigenvalue would be discovered on trying to find V_2 . (See here the remarks at the conclusion of § 1.)

It may be noted that the iterative procedure of this section is closely related to the ordinary method of matrix iteration for the latent vectors of a matrix. We can, in fact, write our procedure as

$$V_{k+1} = (A - \Lambda B)^{-1} B V_k, \tag{16}$$

which, as is well known, leads to convergence to a multiple of that eigenvector, X_p , of (1) for which $|\lambda_p - \Lambda|$ is a minimum.

4. AN ITERATIVE PROCEDURE WITH CUBIC CONVERGENCE

In the foregoing procedures we fixed first the residuals, R , and then the scalars, Λ , in equation (3). We now investigate a combination procedure in which both R and Λ are adjusted at each step. The process is begun with a choice of initial vector V_0 . The succeeding steps are described by the following recursion formulae:

$$R_{k+1} = B V_k \quad (k = 0, 1, 2, \dots), \tag{17}$$

$$\Lambda_{k+1} = \frac{V_k' A V_k}{V_k' B V_k} \quad (k = 0, 1, 2, \dots), \tag{18}$$

$$R_{k+1} = (A - \Lambda_{k+1} B) V_{k+1} \quad (k = 0, 1, 2, \dots). \tag{19}$$

To study the convergence we take

$$V_k = \sum_{i=1}^n c_i X_i \tag{20}$$

with $|c_i/c_p| < \epsilon$ ($i \neq p$). Then from (17) and (18) and the well-known property of Rayleigh's quotient we have

$$\Lambda_{k+1} = \lambda_p + O(\epsilon^2). \tag{21}$$

Inserting (21) into (19) and using (6) we find

$$V_{k+1} = \frac{c_p}{O(\epsilon^2)} \left[X_p + \sum_{i=1}^n \left(\frac{c_i}{c_p} \right) \frac{O(\epsilon^2)}{\lambda_i - \Lambda_{k+1}} X_i \right]. \quad (22)$$

Thus if V_k differs from X_p by terms of order ϵ , V_{k+1} differs from a multiple of X_p by terms of order ϵ^3 . Their Rayleigh quotients have errors of order ϵ^2 and ϵ^6 respectively.

The behaviour of this process in the large is fairly simple. The ordinary behaviour of the method results in sequences of Λ_k and V_k which approach respectively an eigenvalue λ_p and its corresponding mode, X_p . The sequence of Λ_k becomes monotonic after a finite number of steps. This may be seen by considering that each succeeding Λ_k is a weighted average of the λ_i in which the weights for Λ_{k-1} have been increased in proportion to the inverse square of the distance from Λ_{k-1} to the corresponding λ_i . The argument is similar to that made in § 2.

It is possible that after a finite number of steps the sequence of Λ_k may terminate. Although the probability of this is zero, there are several possibilities: (a) Λ_k may be an eigenvalue λ_p , such that $V'_{k-1} B X_p \neq 0$, in which case attempting to find V_k would reveal that Λ_k was an eigenvalue. (b) Λ_k may be midway between two eigenvalues λ_p and λ_q and V_{k-1} has the form $cX_p \pm cX_q$, in which case the sequence of V_k oscillates between multiples of $X_p + X_q$ and $X_p - X_q$ with no alteration in succeeding Λ_k . For this case to arise it would be necessary to choose V_0 at the start in the special form $cX_p \pm cX_q$. There are at most $n(n-1)$ normalized vectors having this form. These vectors may be considered as unstable foci for the process, for if V_0 is taken nearly, but not exactly, in the above form, the process diverges from the oscillating behaviour and eventually converges in the normal fashion. (c) Λ_k may be the common midpoint of $m+1$ pairs of eigenvalues, i.e.

$$\lambda_{p+m} < \dots < \lambda_{p+1} < \lambda_p < \Lambda_k < \lambda_q < \lambda_{q+1} < \dots < \lambda_{q+n}$$

with

$$\lambda_{q+r} - \Lambda_k = \Lambda_k - \lambda_{p+r} \quad \text{for } r = 0, 1, \dots, m$$

and, furthermore, V_{k-1} has the form

$$V_{k-1} = \sum_{r=0}^m c_r (X_{p+r} \pm X_{q+r}).$$

In this case there would be no alteration in succeeding Λ_k , but the sequence of V_k would show oscillating convergence toward multiples of $X_p + X_q$ and $X_p - X_q$. In general, this behaviour occurs only if V_0 is initially of the above special form although the possibility exists that if $V'_0 B X_p = 0$, some subsequent Λ_k might be exactly λ_p , thereby introducing an arbitrary component of X_p into V_k which might leave V_k in the above special form. (See the remarks at the conclusion of § 1.)

5. CONCLUSIONS PERTINENT TO THE RELAXATION METHOD

I have described three iterative procedures constructed within the framework of the relaxation method for eigenvalue problems. In contrast to some iterative procedures these methods exhibit identical convergence characteristics towards all modes. In all three cases convergence can be obtained toward any mode, X_p , of

(1) by appropriate choice of the initial values of Λ , V and R . For example, using the method of § 3, it would only be necessary to choose Λ nearer to λ_p than to any other λ_i and to start with a trial vector V_0 for which $V_0' B X_p \neq 0$. In applying this particular method one way of ascertaining that there would be no tendency toward convergence back to previously determined modes is to orthogonalize the trial vector, V_0 , with respect to these known modes. However, this is clearly unnecessary. For any initial trial vector (which is not simply a linear combination of the previously determined modes) a new eigenvector can always be isolated by trying a finite number of Λ 's. In the methods of §§ 2 and 4, convergence to X_p is expedited if V_0 is already a rough approximation to X_p , but it is obviously unnecessary for V_0 to be orthogonal to any of the other modes.

The relaxation method differs from the iterative procedures described herein in that instead of using (3) to determine V from given Λ and R , in relaxation we control V directly and use (3) to define R . Instead of being bound to a fixed procedure, we are free to make alterations in V as we please. From the preceding analysis it is possible to infer the following guiding principles to aid the relaxation computer in choosing his tactics. During the early exploratory stages of the computation, the alterations in V should be aimed at making R and BV roughly proportional (V is of course an eigenvector if R and BV are exactly proportional). When it becomes clear that this procedure is leading to a vector which is not one of the modes already known, it will probably pay to re-compute Λ and to follow a course in which alterations of V to make R and BV more nearly proportional are alternated with re-computations of Λ . This would achieve the same sort of convergence as our iterative procedure of § 4.

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