

# Separation of Close Eigenvalues of a Real Symmetric Matrix<sup>1</sup>

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In order to test two methods, one proposed by C. Lanczos and the other by M. R. Hestenes and W. Karush, for the numerical calculation of eigenvalues of symmetric matrices, an 8 by 8 matrix is constructed that has several sets of eigenvalues close together. The application of the two methods to this test matrix is described, and in addition, a third method for dealing with such problems is proposed.

In recent publications<sup>2,3</sup> two methods have been proposed for finding eigenvalues of real symmetric matrices. In order to make a numerical comparison between the methods, an 8 by 8 matrix was especially designed (see appendix 1) and the two methods were used independently to get all eight eigenvalues and eigenvectors of the matrix. In order that the test be a severe one, the matrix was designed with several sets of eigenvalues very close together. In order to separate these eigenvalues, special modifications of the two methods were developed for the separation of close eigenvalues (see appendixes 2 and 3).

The method of Lanczos (see footnote 2 and appendix 2) seems best adapted for use by a hand computer using a desk computing machine. In the present case, the computation according to Lanczos' method was carried out by a hand computer, and required of the order of 100 hours computing time.

The method of Hestenes and Karush (see footnote 3 and appendix 3) seems best adapted for use by machine computation. In the present case, the computation according to the method of Hestenes and Karush was carried out on an IBM Card-Programmed Electronic Calculator. Considerable time was spent by Karush in becoming familiar with the machine, so that it is difficult to say just how long the computation would require of an experienced operator. Probably 3 or 4 days would be ample.

During and since the computations described above, there has been much discussion of the problem of separating close eigenvalues of a real symmetric matrix. Besides the methods offered in appendixes 2 and 3, we wish to offer the following modifications of the familiar power method.

First let us consider the case where only the numerically largest eigenvalue,  $\lambda_1$ , and the corresponding eigenvector,  $v_1$ , of a matrix  $A$  are desired. We may assume  $\lambda_1$  to be positive, since otherwise we treat  $-A$ .

Suppose  $\lambda_1, \dots, \lambda_n$  are the eigenvalues of  $A$  in decreasing order, and  $v_1, \dots, v_n$  are the corresponding eigenvectors. If no other eigenvalue is near  $\lambda_1$ , one can find  $\lambda_1$  and  $v_1$  by the standard power method. In order to be able to compare the modi-

fications for the case where another eigenvalue is near  $\lambda_1$ , we review the power method.

First, one chooses a vector  $x$ . This has a representation

$$x = c_1 v_1 + c_2 v_2 + \dots + c_n v_n,$$

but as yet we do not know the  $c$ 's or  $v$ 's. By iterations of the step of operating on a vector with a matrix, we form  $Ax, A^2x, A^3x, \dots$ . The representation of  $A^N x$  is

$$A^N x = c_1 \lambda_1^N v_1 + c_2 \lambda_2^N v_2 + \dots + c_n \lambda_n^N v_n.$$

If  $c_1 \neq 0$  (which is the case except in very extraordinary circumstances), then for sufficiently large  $N$ ,  $c_1 \lambda_1^N$  will be much greater than  $c_i \lambda_i^N$  ( $i > 1$ ), since  $\lambda_1 > |\lambda_i|$  ( $i > 1$ ). Thus  $A^N x$  is nearly a multiple of  $v_1$ . By normalizing in the desired fashion, an approximation (of any desired degree of accuracy) for  $v_1$  is obtained, from which an approximation to  $\lambda_1$  can be obtained.

In case  $\lambda_2 = \lambda_1$ , any linear combination of  $v_1$  and  $v_2$  will serve perfectly well as an eigenvector corresponding to  $\lambda_1$ . The power method just outlined will yield a linear combination of  $v_1$  and  $v_2$  in such a case, and so no difficulty arises.

Suppose  $\lambda_2$  is nearly as great as  $\lambda_1$ , but all other  $\lambda$ 's are appreciably smaller. Then one will have to take  $N$  excessively large before  $c_2 \lambda_2^N$  is small compared to  $c_1 \lambda_1^N$ . Two possible procedures for curtailing the labor are as follows.

In the first, we take  $N$  large enough so that  $c_i \lambda_i^N$  is small compared to  $c_1 \lambda_1^N$  or  $c_2 \lambda_2^N$  for  $i > 2$ . Then approximately,

$$A^N x = c_1 \lambda_1^N v_1 + c_2 \lambda_2^N v_2.$$

Choose two vectors  $y$  and  $z$ . Put

$$a_{2j} = (y, A^{N+j-1}x)$$

$$a_{3j} = (z, A^{N+j-1}x),$$

where  $(u, v)$  denotes the inner product of the vectors  $u$  and  $v$ . Then  $\lambda_1$  and  $\lambda_2$  are the two roots of the quadratic equation

$$\begin{vmatrix} 1 & a_{21} & a_{31} \\ \lambda & a_{22} & a_{32} \\ \lambda^2 & a_{23} & a_{33} \end{vmatrix} = 0. \quad (1)$$

<sup>1</sup> The preparation of this paper was sponsored (in part) by the Office of Naval Research.

<sup>2</sup> C. Lanczos, An iteration method for the solution of the eigenvalue problem of linear differential and integral operators, J. Research NBS 45, 255 (1950) RP2133.

<sup>3</sup> M. R. Hestenes and W. Karush, A method of gradients for the calculation of the characteristic roots and vectors of a real symmetric matrix, J. Research NBS 47, 45 (1951) RP2227.

To prove this, write

$$a = (y, c_1 \lambda_1^N v_1)$$

$$b = (z, c_1 \lambda_1^N v_1)$$

$$c = (y, c_2 \lambda_2^N v_2)$$

$$d = (z, c_2 \lambda_2^N v_2).$$

Then

$$\begin{vmatrix} 1 & a_{21} & a_{31} \\ \lambda & a_{22} & a_{32} \\ \lambda_2 & a_{23} & a_{33} \end{vmatrix} = \begin{vmatrix} 1 & 1 & 1 \\ \lambda & \lambda_1 & \lambda_2 \\ \lambda^2 & \lambda_1^2 & \lambda_2^2 \end{vmatrix} \times \begin{vmatrix} 1 & 0 & 0 \\ 0 & a & b \\ 0 & c & d \end{vmatrix}.$$

Then clearly the determinant is zero whenever  $\lambda = \lambda_2$  or  $\lambda = \lambda_1$ , so that  $\lambda_1$  and  $\lambda_2$  are roots of (1).

In exceptional cases, the coefficients of (1) are all zero. This can happen if  $\lambda_1 = \lambda_2$ , or  $c_1 = 0$ , or  $c_2 = 0$ , or in case the projections of  $y$  and  $z$  are not independent on the subspace spanned by  $v_1$  and  $v_2$  (this is the case where

$$\begin{vmatrix} a & b \\ c & d \end{vmatrix} = 0,$$

and can generally be treated by merely choosing a different  $y$  and  $z$ ).

The case where  $\lambda_1$ ,  $\lambda_2$ , and  $\lambda_3$  are all nearly equal but the remaining  $\lambda$ 's are small can be handled similarly, and leads to a third-degree equation defined by a fourth-order determinant.

Returning to the case where  $\lambda_1$  and  $\lambda_2$  are nearly equal, and other  $\lambda$ 's are smaller, an alternative procedure makes use of Chebyshev polynomials. Suppose that a sufficiently high value of  $N$  has been used in order to establish that there are one or more roots in the vicinity of some value  $\mu$  (which is approximately  $\lambda_1$ , and hence also approximately  $\lambda_2$ , since  $\lambda_1$  and  $\lambda_2$  are nearly equal), and that the other roots are appreciably less than  $\mu$  in absolute value. In particular,  $-\mu$  is a lower bound for the roots. Now instead of taking powers of  $A$ , we take powers of a polynomial in  $A$ , noting that

$$(P(A))^N x = c_1 (P(\lambda_1))^N v_1 + \dots + c_n (P(\lambda_n))^N v_n.$$

If now we choose  $P(\lambda)$  so that  $P(\lambda_1)$  and  $P(\lambda_2)$  are near 1, and  $P(\lambda)$  has a large slope in the neighborhood of  $\lambda_1$  and  $\lambda_2$ , then  $P(\lambda_1)$  and  $P(\lambda_2)$  will have a ratio appreciably less than  $\lambda_1/\lambda_2$ , and hence powers of  $P(A)$  will eliminate  $v_2$  relative to  $v_1$  faster than powers of  $A$ .

We first apply  $A$  enough times to eliminate all  $v$ 's except  $v_1$  and  $v_2$ , and then apply  $P(A)$ . In order to insure that  $P(A)$  does not bring back the  $v$ 's already eliminated, it suffices that  $|P(\lambda)| \leq 1$  for  $-\mu \leq \lambda \leq \mu$ . To do this and simultaneously maximize the slope of  $P(\lambda)$  at  $\lambda = \mu$  for  $P(\lambda)$  a polynomial of degree  $M$ , it suffices to take

$$P(\lambda) = T_M \left( \frac{\lambda}{\mu} \right),$$

where  $T_M$  is the Chebyshev polynomial of degree  $M$ .<sup>4</sup>

Actually, it may be more efficient to use different polynomials at different stages in the proceedings. The optimum choices of the polynomials will depend on the distribution of the  $\lambda$ 's, naturally. As this is not known ahead of time in a given case, one must depend on a combination of experience and alert improvisation to get a good choice of polynomials.

We now turn to the case where one wishes to find all eigenvalues and eigenvectors. If any sort of fast computing machinery is available, one can probably proceed best by a combination of the power method plus orthogonalization on the eigenvectors already known. In particular, suppose  $\lambda_1$  and  $v_1$  are known. We can start with  $x$  and orthogonalize it with respect to  $v_1$ . That is, we replace  $x$  by

$$x - \frac{(v_1, x)}{(v_1, v_1)} v_1.$$

For the resulting vector, we have  $c_1 = 0$ . Hence, if we apply powers of  $A$  to it, we get the eigenvector corresponding to the eigenvalue next greatest after  $\lambda_1$  in absolute value. Unfortunately, since we do not know  $v_1$  exactly, we cannot in general determine  $x$  to be exactly orthogonal to  $v_1$ , and so cannot insure  $c_1 = 0$ . We thus face the possibility that  $c_1 \lambda_1^N$  may again be large. If, however, we orthogonalize with respect to  $v_1$  from time to time, we repeatedly cut down the size of  $c_1 \lambda_1^N$ . On a fast machine, orthogonalization is a quick procedure, and it is probably worthwhile to alternate the steps of orthogonalization and operating with  $A$ .

If  $\lambda_1$  and  $\lambda_2$  and  $v_1$  and  $v_2$  are known, one orthogonalizes with respect to both  $v_1$  and  $v_2$  between each time that one operates with  $A$ .

If at any point in the procedure, one encounters two close eigenvalues, one is trying to find the largest unknown eigenvalue, and so can apply the methods noted above (which are not disturbed by the frequent orthogonalizations). However, now that one plans to find all eigenvalues, alternative quicker methods are available for separation of close eigenvalues, depending upon knowing all other eigenvalues and eigenvectors. For example, suppose  $A$  has eigenvalues 1, 2, 2.95, 3.05, 4, and 5. Successively getting the largest eigenvalue twice by the power method plus orthogonalization, we readily get the eigenvalues 5 and 4, and their eigenvectors. We now discover that there are troubles in the neighborhood of 3. Essentially, we "postpone" treatment of this point by putting  $B = 3I - A$ . Then the eigenvalues 1, 2, 2.95, 3.05 of  $A$  lead to the eigenvalues 2, 1, 0.05, -0.05 of  $B$ . Going now for the largest eigenvalues of  $B$ , we quickly get 2 and 1. We now have all eigenvalues and eigenvectors of  $A$  except 2.95 and 3.05 and their eigenvectors. Also we now know that there are just two remaining eigenvalues, and that both are near 3. We now consider  $C = A - 2.9I$ . This has eigenvalues 0.05 and 0.15, and the power

<sup>4</sup> G. Pólya and G. Szegő, *Aufgaben und Lehrsätze aus der Analysis* 11, p. 91 (Dover Publications, New York, N. Y., 1945).

method plus orthogonalization quickly gives the larger of these.

This method will run into difficulties if there are two pairs of close eigenvalues. An alternative procedure that will take care even of this case is the following. Suppose we have eigenvalues  $\lambda_1=5$ ,  $\lambda_2=4.05$ ,  $\lambda_3=3.95$ ,  $\lambda_4=3$ ,  $\lambda_5=2.05$ ,  $\lambda_6=1.95$ , and  $\lambda_7=1$ . We quickly find  $\lambda_1$  and  $v_1$ . Trying for  $\lambda_2$ , we find trouble. By starting with some  $x$  and alternately orthogonalizing with respect to  $v_1$  and operating with  $A$ , we keep  $v_1$  out, and eventually eliminate  $v_4$ ,  $v_5$ ,  $v_6$ , and  $v_7$ . We now have a certain linear combination of  $v_2$  and  $v_3$ , which we may as well call  $u_2$ . We now repeat the procedure, except for starting with a different  $x$ . We then get a  $u_3$  that is also a linear combination of  $v_2$  and  $v_3$ . Except in the most extraordinarily unfortunate cases,  $u_3$  will be independent of  $u_2$ . One can insure this independence by orthogonalizing with respect to  $u_2$  throughout the computation of  $u_3$ . However, it is scarcely worth while, except perhaps in the choice of the initial  $x$ .

Since  $u_2$  and  $u_3$  are independent linear combinations of  $v_2$  and  $v_3$ , it follows that a vector is orthogonal to both of  $v_2$  and  $v_3$  if and only if it is orthogonal to both of  $u_2$  and  $u_3$ . To find  $\lambda_4$  and  $v_4$ , we would wish to orthogonalize with respect to all of  $v_1, v_2, v_3$ . We can get the same effect if we instead orthogonalize with respect to  $v_1, u_2$ , and  $u_3$  (this is most conveniently done if  $u_3$  is taken orthogonal to  $u_2$ ). Thus we can now proceed to get  $\lambda_4$  and  $v_4$ , although we do not yet know  $\lambda_2, \lambda_3, v_2$ , or  $v_3$ . We again encounter difficulty with  $v_5$ , and  $v_6$  because  $\lambda_5$  and  $\lambda_6$  are near together. However, we can get a  $u_5$  and a  $u_6$ , which will suffice to let us obtain  $\lambda_7$  and  $v_7$ . Now, by orthogonalizing with respect to  $v_1, v_4, u_5, u_6$ , and  $v_7$ , we can readily separate  $\lambda_2$  and  $\lambda_3$  by working with powers of  $A-3.9I$ . Then we get  $\lambda_5$  and  $\lambda_6$  by working with powers of  $A-1.9I$ .

## Appendix 1. Construction of a Test Matrix

In order to get eigenvalues very close together without using many significant digits in the coefficients, it seemed necessary to use irrational numbers. Accordingly, a search was made for 2 by 2 symmetric matrices with eigenvalues, some of which were near together. We decided on the following four, where the eigenvalues are written to the right of the matrices:

$$\begin{array}{l} \left\| \begin{array}{cc} 102 & 1 \\ 1 & -102 \end{array} \right\| \quad \pm \sqrt{(102)^2+1} \\ \left\| \begin{array}{cc} 101 & 1 \\ 1 & 101 \end{array} \right\| \quad 101 \pm 1 \\ \left\| \begin{array}{cc} 1 & 10 \\ 10 & 101 \end{array} \right\| \quad 51 \pm \sqrt{(51)^2-1} \\ \left\| \begin{array}{cc} 98 & 14 \\ 14 & 2 \end{array} \right\| \quad 100, 0 \end{array}$$

The approximate numerical values of these eight eigenvalues, written in descending order are:

102.005  
102.000  
101.990  
100.000  
100.000  
0.010  
0.000  
-102.005

One eigenvalue, namely 100, is exactly repeated. These 2 by 2 matrices were then mixed together into an 8 by 8 matrix as follows:

$$\left\| \begin{array}{cccccccc} 102 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 101 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 98 & 0 & 0 & 0 & 14 & 0 \\ 0 & 0 & 0 & 1 & 10 & 0 & 0 & 0 \\ 0 & 0 & 0 & 10 & 101 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & -102 & 0 & 0 \\ 0 & 0 & 14 & 0 & 0 & 0 & 2 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 101 \end{array} \right\|$$

Temporarily call this matrix  $B$ , and let  $P$  denote

$$\left\| \begin{array}{cccccccc} 2 & 1 & 1 & 2 & 0 & 0 & 0 & 0 \\ 1 & -2 & -2 & 1 & 0 & 0 & 0 & 0 \\ 1 & 2 & -2 & -1 & 0 & 0 & 0 & 0 \\ 2 & -1 & 1 & -2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & -1 & -2 & 2 \\ 0 & 0 & 0 & 0 & -1 & -1 & 2 & 2 \\ 0 & 0 & 0 & 0 & -2 & -2 & -1 & -1 \\ 0 & 0 & 0 & 0 & 2 & -2 & 1 & -1 \end{array} \right\|$$

The two 4 by 4 matrices occurring in the corners of  $P$  were made by a scheme due to Sylvester,<sup>5</sup> with the result that  $P$  has the property

$$P^T P = 10I$$

(we use  $P^T$  to denote the transpose of  $P$ ). We then defined  $A$  to be  $P^T B P$ . The matrix  $A$  is then

$$\left\| \begin{array}{cccccccc} 611 & 196 & -192 & 407 & -8 & -52 & -49 & 29 \\ 196 & 899 & 113 & -192 & -71 & -43 & -8 & -44 \\ -192 & 113 & 899 & 196 & 61 & 49 & 8 & 52 \\ 407 & -192 & 196 & 611 & 8 & 44 & 59 & -23 \\ -8 & -71 & 61 & 8 & 411 & -599 & 208 & 208 \\ -52 & -43 & 49 & 44 & -599 & 411 & 208 & 208 \\ -49 & -8 & 8 & 59 & 208 & 208 & 99 & -911 \\ 29 & -44 & 52 & -23 & 208 & 208 & -911 & 99 \end{array} \right\|$$

<sup>5</sup> T. Muir, History of determinants III, 289 (Macmillan and Co., Ltd., London, 1920).



appears in the following symmetric form:

$$C' = \begin{pmatrix} \alpha_0 & \gamma_1 & & & \\ \gamma_1 & \alpha_1 & \gamma_2 & & \\ & \gamma_2 & \alpha_2 & \gamma_3 & \\ & & & \ddots & \\ & & & & \gamma_{n-1} & \alpha_{n-1} \end{pmatrix} \quad (10)$$

The quantities  $\alpha_i$  and  $\beta_i$ , obtained by the method of minimized iterations, contain the entire solution of the eigenvalue problem. The eigenvalues are contained in the solution of the algebraic equation (4), while the components of the eigenvector  $u_i$ , analyzed in the  $b_i$ -system, become:

$$p_0(\lambda_i), p_1(\lambda_i), \dots, p_{n-1}(\lambda_i). \quad (11)$$

If we construct the matrix

$$P = \begin{pmatrix} p_0(\lambda_1), p_1(\lambda_1), \dots, p_{n-1}(\lambda_1) \\ \vdots \\ p_0(\lambda_n), p_1(\lambda_n), \dots, p_{n-1}(\lambda_n) \end{pmatrix} \quad (12)$$

then the matrix product

$$U = PB. \quad (13)$$

where  $B$  is the matrix of the  $b_i$ , gives the matrix of the eigenvectors  $u_i$ , associated with the original matrix  $A$ .

The orthogonality of the eigenvectors  $u_i$  finds expression in the following relation:

$$1 + \sum_{\alpha=1}^{n-1} \frac{p_\alpha(\lambda_i) p_\alpha(\lambda_j)}{\beta_1 \beta_2 \dots \beta_\alpha} = 0 \quad (i \neq j) \quad (14)$$

In the given test-matrix a preliminary investigation of the matrix revealed that the largest eigenvalue is of the order of magnitude  $\pm 1000$ . Hence all the elements of  $A$  were divided by 1000, thus obtaining a new matrix

$$A_0 = \frac{A}{1000},$$

whose largest eigenvalue was of the order  $\pm 1$ .

The trial vector  $b_0$  was chosen to be

$$0, 1, 0, 0, \dots, 0$$

Then the method of minimized iterations was applied, obtaining the  $B$  matrix by putting the components of the vectors  $b_0, b_1, b_2, \dots, b_{n-1}$  in successive rows. Each one of these vectors was corrected during the process of generation to become strictly orthogonal to the previous vectors. Hence  $b_n$  must come out as identically zero, in spite of rounding errors. The associated  $\alpha_i$  and  $\beta_i$ , together with the  $\gamma_i = \sqrt{\beta_i}$ , are tabulated as follows:

$i$	$\alpha_i$	$\beta_i$	$\gamma_i$
0	0.899		
1	.1086629633	0.096939	0.3113502850
2	.7859177671	.039517948848	.03085117315
3	-.7935214279	.4088977136	.6394511034
4	.003963315517	.0520498144977	.001431717325
5	1.0160663075	.004021099703	.06341214161
6	1.0199110708	.01070421101	.03271729055
7	1.0000000030	.017048359779	.08395451018

We will now discuss the problem of obtaining the roots of the algebraic equation (4). Our procedure will be to obtain a good first approximation and then improve this approximation to the full accuracy obtainable by 10 digit calculations.<sup>7</sup>

The separation of nearly equal roots is frequently a rather cumbersome task. In the present method the existence of nearly equal roots is an asset rather than a liability. The orthogonality relation (14) shows that exactly equal or nearly equal roots are only possible under singular conditions. If none of the  $\beta_i$  are small, then  $\lambda_i$  and  $\lambda_j$  cannot be essentially equal since a sum of all positive terms cannot vanish. If, on the other hand, a certain  $\beta_i$  is zero or very small, this means that the polynomial  $p_n(x)$  separates into the product of two independent polynomials of lower order, which greatly simplifies the evaluation of the roots.

The given numerical example is well adapted to demonstrate the behavior of equal or nearly equal roots. Since nearly equal roots operate as practically one root in the successive reduction of the trial vector  $b_0$ , we will obtain a very small  $b_m$  already after  $m$  steps, where  $m$  is the number of essentially different roots. In the present problem we have only three essentially different roots. Owing to an accidental degeneracy, only two of these roots were strongly represented in  $b_0$ . Hence  $\beta_2$  is already small. The remaining vector again contained essentially but two roots, and thus  $\beta_1$  is again small. Furthermore, we notice that  $\beta_6$  is very small and  $\beta_7$  almost negligible.

Indeed, the fact that two roots of the given problem coincide has the consequence that  $b_0$  should get reduced to zero in already seven steps, thus making  $\beta_7$  exactly zero. That  $\beta_7$  is not exactly zero, but only to 9 decimal places, is due to rounding errors.

The associated  $\alpha_7$  should give the double root  $\lambda=1$ . Actually

$$\alpha_7 = 1.0000000030$$

is a very close approximation of the exact root.

We also notice that already  $\beta_6$  is very small, although 15 times larger than  $\beta_7$ . The associated

$$\alpha_6 = 1.0199110708$$

is a close approximation of another of the nearly equal roots, namely

$$\lambda = 1.0199019514.$$

These specific properties of the  $\beta_i$  have the consequence that the original equation of 8th order separates into equations of the order

$$2+2+2+1+1.$$

This yields eight approximate roots of our problem, without solving equations of higher than second order.

The question is now, how to improve the accuracy of these approximations. The application of Newton's method for correcting a root is here out of question since we cannot construct the actual polynomial  $p_8(x)$  without such rounding errors, which completely annihilate the desired accuracy. We can construct the successive polynomials  $p_i(\lambda)$  for any given  $\lambda$  by the recurrence relations (2), but for arbitrary  $\lambda$  the coefficients of the final polynomial are marred by intolerably large errors.

The following perturbation method has quick convergence and operates numerically very satisfactorily. Let us assume that we possess a vector  $y$ , which approximates the solution of the eigenvalue problem.

$$Ay - \lambda y = 0. \quad (15)$$

Then

$$\lambda = \frac{yAy}{y^2} \quad (16)$$

is a very satisfactory approximation of a certain  $\lambda_i$ , because an error of first order in  $y$  causes an error of only second order in  $\lambda$ .

<sup>7</sup> This means 10 decimal places if the largest eigenvalue is normalized to 1. The absolutely smallest eigenvalue may be zero or arbitrarily near to zero. This zero, however, cannot be ascertained to more than 10 decimal places. The relative accuracy of the smallest eigenvalue may thus become arbitrarily bad.

We will apply this principle to our problem in the following sense. Let us assume that  $\bar{\lambda}$  is an approximate root of the polynomial  $p_n(\lambda)$ . We now construct the components of the vector  $y$  by evaluating the following recurrent sequence:

$$\begin{aligned} y_0 &= 1 \\ y_1 &= \frac{(\bar{\lambda} - \alpha_0)y_0}{\gamma_1} \\ y_2 &= \frac{(\bar{\lambda} - \alpha_1)y_1 - \gamma_1 y_0}{\gamma_2} \\ &\vdots \\ y_{n-1} &= \frac{(\bar{\lambda} - \alpha_{n-2})y_{n-2} - \gamma_{n-2}y_{n-3}}{\gamma_{n-1}} \\ y_n &= (\bar{\lambda} - \alpha_{n-1})y_{n-1} - \gamma_{n-1}y_{n-2}. \end{aligned} \quad (17)$$

The vector

$$y = (y_0, y_1, \dots, y_{n-1}) \quad (18)$$

taken in the reference system of the  $b'_i$ , satisfies the equation

$$Ay - \bar{\lambda}y = 0$$

in all its components except the *last* one, where we get

$$(Ay - \bar{\lambda}y)_{n-1} = -y_n.$$

Hence

$$yAy = \bar{\lambda}y^2 - y_n y_{n-1}.$$

Substitution in (16) gives

$$\lambda = \bar{\lambda} - \frac{y_n y_{n-1}}{\sum y_i^2}$$

Actually it is entirely accidental that the equation where the error occurs shall be the *last* one. We can start our recurrences from *both* ends of the matrix and join the two sets at an arbitrary point  $i$ . The error will then occur in the  $i$ th rather than the last equation.

Now the correction of the error of  $\bar{\lambda}$  will be most effective if the error of the equation (15) appears in that particular component  $i$  that is associated with the absolutely largest  $y_i$ . We designate this particular  $y_i$  and add to the sequence (17) another sequence that starts from the other end and proceeds in opposite direction:

$$\begin{aligned} y'_{n-1} &= 1 \\ y'_{n-2} &= \frac{(\bar{\lambda} - \alpha_{n-1})y'_{n-1}}{\gamma_{n-1}} \\ y'_{n-3} &= \frac{(\bar{\lambda} - \alpha_{n-2})y'_{n-2} - \gamma_{n-1}y'_{n-1}}{\gamma_{n-2}} \\ &\vdots \\ y'_{i-1} &= \frac{(\bar{\lambda} - \alpha_i)y'_i - \gamma_{i+1}y'_{i+1}}{\gamma_i} \end{aligned} \quad (19)$$

We adjust this sequence to the sequence (17) by multiplying every component by

$$\rho = \frac{y_i}{y'_i}. \quad (20)$$

We now construct our vector  $y$  by choosing its components from the  $y_k$  series up to  $k=i$ , and from the  $y'_k$  series from

$k=i$  on:

$$\left. \begin{aligned} \bar{y}_0 &= y_0, \bar{y}_1 = y_1, \dots, \bar{y}_i = y_i = \rho y'_i \\ \bar{y}_{i+1} &= \rho y'_{i+1}, \dots, \bar{y}_{n-1} = \rho y'_{n-1} \end{aligned} \right\} \quad (21)$$

The error occurs in the  $i$ th equation and we obtain

$$\lambda = \bar{\lambda} + \frac{\gamma_i(y_{i-1} - \rho y'_{i-1})y_i}{\sum \bar{y}_\alpha^2}. \quad (22)$$

The entire process can now be repeated, by replacing  $\bar{\lambda}$  by the new  $\lambda$ . This process had such good convergence that after two steps the error was already pushed out beyond the 10th decimal place. The entire set of  $\lambda_i$  was thus obtained with relatively little difficulty and without involved calculations.

After obtaining the  $\lambda_i$ , the  $P$  matrix was obtained by recursions. Finally, the product  $PB$  gave the matrix  $U$  of the eigenvectors  $u_i$ . This matrix was then normalized by dividing each row by the square root of the sum of the squares of the elements of each row.

The resultant normalized matrix  $U'$  was now tested for orthogonality and for its eigenvector property. Under exact conditions we should get

$$u'_i u'_k = 0 \quad (i \neq k) \quad (23)$$

$$u'_i A u'_k = 0 \quad (i \neq k)$$

Actually, in view of the rounding errors, we do not get zero on the right side but two symmetric matrices

$$\rho_{ik} = \rho_{ki} \quad (24)$$

and

$$\sigma_{ik} = \sigma_{ki} \quad (25)$$

composed of small elements. We use these  $\rho_{ik}$  and  $\sigma_{ik}$  quantities to correct our solution. We evaluate

$$\epsilon_{ik} = \frac{\sigma_{ik} - \lambda_i \rho_{ik}}{\lambda_i - \lambda_k}. \quad (26)$$

In view of the extreme closeness of some of the eigenvalues, the denominator of (26) becomes small for some  $i, k$ , and the corresponding  $\epsilon_{ik}$  not negligible. We now form the matrix  $E$ , composed of the non-negligible elements  $\epsilon_{ik}$ , while the diagonal elements and the negligible  $\epsilon_{ik}$  are replaced by zero. The corrected  $U'$  matrix becomes:

$$\bar{U}' = U' + E U' \quad (27)$$

The rows of the corrected matrix give us the proper eigenvectors with an accuracy of six decimal places. The  $\lambda_i$ , evaluated from these vectors, agreed with the previous  $\lambda_i$  to 10 decimal places. Comparison with the known exact values showed that all the 10 decimal places came out correctly for each one of the roots.<sup>8</sup>

### Appendix 3. Modification of the Method of Hestenes and Karush

The method of fixed  $\alpha$  (see footnote 3) was used in the calculation. This consists in passing from one approximation  $x$  for a characteristic vector to the next approximation  $x'$  by means of the formula

$$x' = x + \alpha \xi(x)$$

where

$$\xi(x) = Ax - \mu(x)x, \quad \mu(x) = \frac{(x, Ax)}{(x, x)}.$$

Here  $\alpha$  is a positive constant (independent of  $x$ ) of the form

$$\alpha = \frac{\beta}{\lambda_1 - \lambda_n}, \quad 0 < \beta < 1,$$

<sup>8</sup> The entire numerical work was carried out by Miss Fannie M. Gordon.

where  $\beta$  is optimally near 1. The above formula for  $x'$  is used to obtain convergence to an eigenvector  $v_1$  belonging to  $\lambda_1$ , the largest (algebraically) eigenvalue. For an eigenvector  $v_n$  belonging to  $\lambda_n$ , the smallest eigenvalue, the formula

$$x' = x - \alpha \xi(x)$$

is to be used. In practice  $\alpha$  is at the disposal of the computer, and he may change its value at different stages of the calculation according to his disposition and insight. The changes are easily made by having at hand several punched cards carrying different values of  $\alpha$  and replacing at any time the single card in the deck carrying the value of  $\alpha$  by another such card.

The fixed  $\alpha$  method is closely related to the power method. To illustrate this, suppose we are computing the least value  $\lambda_8$ . After a certain number of steps the value of  $\mu(x)$  will be essentially constant from step to step, this constant representing our computed value of  $\lambda_8$ . Continued calculation leads to improvement in the vector  $x$ . The iteration formula with  $\xi(x)$  replaced by its expression in terms of  $Ax$  and  $x$  becomes

$$x' = \alpha \left\{ \left( \frac{1}{\alpha} + \mu \right) I - A \right\} x,$$

with  $I$  the identity matrix. That is, approximately,

$$x' = \alpha \{ (\beta' \lambda_1 + (1 - \beta') \lambda_8) I - A \} x,$$

where  $\beta' = 1/\beta$  is near 1. Thus, except for a normalization factor  $\alpha$ , this is the power method applied to  $\lambda_1 I - A$  with  $\lambda_1'$  near  $\lambda_1$ . In essence we have shifted the origin close to  $\lambda_1$ , thereby making  $\lambda_8$  the dominating eigenvalue in absolute value. The normalizing factor  $\alpha$  guarantees that the lengths  $|x|$  will increase and converge.

The above procedure was used to calculate all eigenvalues and eigenvectors by the technique of orthogonalizing to eigenvectors already known, in the manner described in the text. As more eigenvectors are obtained the parameter  $\alpha$  is allowed to assume a greater value, this value in each new case being of the form  $\beta/M$ , where  $M$  is the spread of the eigenvalues for the subspace in question. Thus if  $\lambda_8$  and  $v_8$  are known, the iteration operates in the 7-dimensional subspace orthogonal to  $v_8$ , where the appropriate value of  $M$  is  $\lambda_1 - \lambda_7$ .

Multiple roots offer no difficulty. Thus in the case of  $\lambda_4 = \lambda_5 = 1000$ , the iteration first leads to the eigenvalue  $\lambda_4 = 1000$  and to some corresponding eigenvectors  $v_4$ . Running orthogonal to  $v_4$  (and other known eigenvectors) we obtain  $\lambda_5 = 1000$  and the eigenvector  $v_5$  orthogonal to  $v_4$ .

Close roots may be treated as follows. At first the close roots are ignored and because  $\lambda_1, \lambda_2, \lambda_3$  are nearly equal and  $\lambda_6, \lambda_7$  are nearly equal one obtains by the orthogonalization technique eight independent vectors

$$u_1, u_2, u_3, v_4, v_5, u_6, u_7, v_8$$

instead of the true eigenvectors

$$v_1, v_2, v_3, v_4, v_5, v_6, v_7, v_8.$$

Here  $u_1, u_2, u_3$  are linear combinations of  $v_1, v_2, v_3$  and  $u_6, u_7$  are linear combinations of  $v_6, v_7$  (see text). To find the first vector  $v_1$  we apply our iteration procedure in the 3-space spanned by these vectors. That is, we run orthogonal to  $v_4, v_5, u_6, u_7, v_8$  and use a (large)  $\alpha$  appropriate to the 3-space. Having obtained  $v_1$  we run orthogonal to  $v_1$  to obtain  $v_2$ . To obtain  $v_3$  we do not require the  $\alpha$  iteration method; we need only orthogonalize to  $v_1$  and  $v_2$  in the 3-space. Notice that this procedure of obtaining  $v_1, v_2, v_3$  does not require knowing  $u_1, u_2, u_3$ . Of course if one decided to separate  $v_6$  and  $v_7$  first, one would need to know these last three vectors but not  $u_6$  and  $u_7$ .

In connection with orthogonalizing to known eigenvectors we remark that if  $x$  is already orthogonal to such vectors then in theory  $x'$  and all successive approximations will be. In practice however the orthogonality is lost by round-off and must be regularly restored by direct calculation.

The preceding method was, in the main, the one used in the computation. However, there is a variation of the procedure that is of interest. It takes advantage of the fact that we may make the iteration scheme move upward or downward on the scale of eigenvalues and enables us to reduce the number of orthogonalizations. Consider the problem of finding  $v_1, v_2, v_3$ . We first apply the iteration procedure that increases  $\mu(x)$ , that is,  $x' = x + \alpha \xi$ , with an  $\alpha$  appropriate to the whole space. After a certain number of steps we have eliminated the lower eigenvectors and are operating in the invariant 3-space of  $v_1, v_2, v_3$ . We now increase  $\alpha$  to a value corresponding to the three space. In this way we separate out  $v_1$ . In order to avoid the introduction of higher eigenvectors through round-off, we intersperse use of the larger value of  $\alpha$  with use of the older smaller value (this replaces the orthogonalization to  $v_4, v_5, u_6, u_7, v_8$  of the preceding method). The next vector  $v_2$  is obtained in the same way, maintaining orthogonality to  $v_1$ . The vector  $v_3$  is found by orthogonalizing to  $v_1$  and  $v_2$ . To apply this technique to  $v_6$  and  $v_7$  we first find  $v_8$  and then use the  $\alpha$  iteration with decreasing  $\mu$ , that is,  $x' = x - \alpha \xi$ . Then  $v_7$  is found by orthogonalizing only to  $v_8$ , and  $v_6$  by orthogonalizing to  $v_8$  and  $v_7$ .

If we analyze either of the above methods of separation in the way we earlier compared the fixed  $\alpha$  method with the power method, we find again that in the later stages of the iteration we are applying the power method. We first eliminate all but the invariant subspace corresponding to the close eigenvalues, and then, in essence we use the power method on a linear combination of  $A$  and  $I$  that will separate out the desired vectors. Thus, this method is closely related to that explained at the end of the text.

The final eigenvalues were found with a relative error of  $10^{-8}$ . The absolute in the components of each eigenvector were determined with an absolute error of  $10^{-8}$ , when the largest component of each vector is taken to be 1.

LOS ANGELES, September 28, 1950.