ON AN AUTOMATIC COMPUTATION OF CHARACTERISTIC ROOTS OF A MATRIX

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ABSTRACT

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A method consisting in finding a two dimensional elementary transformation for obtaining eigen values has been discussed with details of programming aspects and it has been shown with the help of numerical examples that this method is as efficient as L-R transformation so far as the number of iteration steps are concerned and moreover, it demands less machine time, less number of arithmetic operations (particularly divisions and multiplications) per iteration and less memory storage. Like L-R transformation this method is always stable for positive d.finite matrices and takes substantially less machine time than Q-R transformation and moreover, can be used both for symmetric and unsymmetric matrices.

INTRODUCTION

Jocobi's iteration method for finding eigen values and eigen vectors of symmetric matrices as revived by Von Neumann¹⁹ for modern large computers, is well known and popular. A Jacobi-like method suggested by Eberlein¹⁶⁻¹⁰ for unsymmetric matrices has a wide range of application, but they require the calculation of several square-root functions in each iteration leading to rounding error and more computational time per iteration. The present method, however, does not involve calcution of aforesaid function thus obviating such rounding error and saving on operational time. It requires simple operations like addition, subtraction, multiplication and division while however utilizing, like the aforesaid methods, the principle of similar transformation. Like L-R transformation the present method also may not work in the case of singular matrices. In the following the method is discussed vis-a-vis L-R transformation stressing the programming aspects. Numerical examples are given to provide illustration. The relative computing time as well as memory requirements and number of arithmetic operations are also indicated.

METHODS

Method 1: (Based on two dimensional elementary transformation). This method consists in finding a sequence of two dimensional elementary transformations E_i such that if $E = \prod_i E_i$ then $E^{-1}AE$ are approximately diagonal with the approximations to the eigen values appearing on the diagonal, where A is a matrix of order n. The E_i which range over all two dimensional subspaces are determined at each step of the iteration to reduce to zero all the *i*-th row elements of A excluding, however, the first *i* elements. The matrix E_k will be an upper triangular¹³ matrix of the form

$$e_{jj} = 1, \quad j = 1, 2, 3, \cdots, n$$

$$e_{ki} = -a_{ki}/a_{kk}, \quad i = k+1, \quad k+2, \quad k+3, \cdots, n-1, n$$

$$e_{pq} = 0, \quad p = 1, 2, 3, \cdots, n-2, \quad n-1; \quad q = p+1, \quad p+2, \cdots, n$$

$$p \neq k$$

and consequently E_k^{-1} is also an upper triangular matrix of the form

$$\begin{aligned} e_{jj} = 1, \quad j = 1, 2, 3, \cdots, n-1, n \\ e_{ki} = a_{ki} / a_{kk}, \quad i = k+1, \quad k+2, \quad k+3, \cdots, n \\ e_{j,i} = 0 \quad p = 1, 2, 3, \cdots, n-2, \quad n-1; \quad q = p+1, \quad p+2, \cdots, n \\ p \neq k \end{aligned}$$

Now

$$E_{k}^{-1}A_{k}E_{k} = A_{k+1}$$
, $A_{1} = A$, $k = 1, 2, 3, \cdots, n-2$, $n-1$

All the matrices A_k , k = i, 2, 3, \cdots , n-2, n-1 will assume the same memory locations as the original matrix A. According to the principle of similar transformation, the roots of A_{k+1} and A_k will be the same. The process will continue till almost all the elements above the left diagonal of A_k turn out to be very small or zero depending on the accuracy desired.

Method 2: (L-R transformation). A square matrix A can be expressed uniquely as the product of a lower triangular matrix L and upper triangular matrix R, provided the diagonal elements of one of these matrices are specified. In this method suggested by Rutishauser¹³, all the diagonal elements of L are taken as 1. If $A = A_1$, we can decompose A_1 into L_1 and R_1 such that $A_1 = L_1 R_1$. The elements of L_1 and R_1 are determined from the original matrix A_1 . We then form the reverse product $R_1 L_1$. It will be different from A_1 . Let it be denoted by A_2 . We can decompose A_2 into L_2 and R_2 such that $A_2 = L_2 R_2$. Similarly $R_2 L_2 = A_3 = L_3 R_3$ and so on, where A_3 is the matrix formed by the product of R_2 and L_2 .

This yields an infinite sequence of matrices A_k . After a large number of steps this process converges resulting in an upper triangular matrix A_k while the lower triangular matrix converges to an identity matrix; the number of transformations required for such convergence depends on the nature of the elements of the original matrix,

This L - R transformation is also a similarity transformation and hence keeps the characteristic equation of A_{i} 's invariant.

PROGRAMMING ASPECIS'

Method 1. (a) Formulae of transformation: The elements of the matrix A_k will be transformed due to the post multiplication of A_k by E_k as

$$a_{ki} = 0 \qquad i = k + 1, \ k + 2, \ k + 3, \ \cdots, n - 1, n \qquad [i]$$

$$a_{ij} = a_{ij} - (a_{kj}/a_{kk}) a_{ik} \qquad [i]$$

$$i = k + 1, \ k + 2, \ k + 3, \ \cdots, n - 1, m$$

$$j = k + 1, \ k + 2, \ k + 3, \ \cdots, n - 1, n$$

and the remaining will remain unchanged. The *a*'s on the *r* h s of [ii] are the elements of A_k throughout the transformation and not in any case the elements of $A_k E_k$.

Now $A_k E_k$ has the same locations as A_k and to find $E_k^{-1} A_k E_k$ we will refer to the elements of A_k , since $A_k = A_k E_k$. Due to the pre-multiplication by E_k^{-1} the transformed elements of A_k (*i.e.* $A_k E_k$) will be

$$a_{kj} = \sum_{p=k+1}^{n} a_{pj} \left(a_{kp} / a_{kk} \right) + a_{l,j}, \quad j \leq k$$
 [iii]

$$a_{kj} = \sum_{p=k+1}^{n} a_{pj} \left(a_{kp} / a_{kj} \right), \qquad j > k \qquad [iv]$$

$$j = 1, 2, 3, \cdots, n - 1, n.$$

The rest of the elements of A_k (*i.e.* $A_k E_k$) will remain unchanged for a particular k. The elements o_{kp}/a_{kk} were the elements of the original matrix A_k *i.e* before the formation of $A_k E_k$. The other elements on the right hand side of [iii] and [iv] were the elements of A_k (*i.e.* $A_k E_k$) and not in any case the elements of $E_k^{-1} A_k$. For a single iteration $k = 1, 2, 3, \dots, n-2, n-1$.

(b) Checks. Trace check is performed

(c) Memory requirements. About $n^2 + n + 65$ words are necessary of which n^2 locations are required for the storage of matrix A of order n, n locations for the storage of one row (or column) of A, and 65 locations for the program.

(d) Computing time per iteration. (referring to formulae i, il, iii, iv)

It is about
$$\sum_{k=1}^{n-1} (n-k) v_1 + 2 \sum_{k=1}^{n-1} (n-k)^2 v_2 + \sum_{k=1}^{n-1} (n-k)^2 v_3 + \left\langle \left[\sum_{k=1}^{n-1} (n-k) (n-k-1) \right] + (n-1) \right\rangle v_4 + \tau_1 (n) \right\rangle$$

* '=' will always mean ' is replaced by ' in discussions under ' Programming Aspects'

where the first 4 terms with v's deleted indicate number of divisions, multiplications, subtractions and additions respectively, and $\tau_1(n)$ is the time needed by input and output units inclusive of that due to logical operations, v_1, v_2, v_3 and v_4 are the division, multiplication, subtraction and addition time respectively.

Method 2. (a) Formulae of L-R transformation: We determine the R and L matrices as follows

R matrix:
$$r_{ij} = a_{ij} \sum_{p=1}^{i-1} l_{ip} r_{pj}$$
, assuming $l_{il} = 1$ (v)

L matrix:
$$l_{ij} = (a_{ij} - \frac{1}{p-1} l_{ip} r_{pj})/r_{jj}$$
 (vi)

For actual computation we assume a fixed value for j (which has to be taken as 1 first) and then proceed varying $i = 1, 2, 3, \dots, n-1, n$ and as a result we find r_{11} , then l_{21} , l_{31} , l_{41} , \cdots , $l_{n-1, 1}$, $l_{n, 1}$ respectively. We then take j = 2 and proceed varying $i = 1, 2, 3, \dots, n-1$, n and as a result we find r_{10} , r_{22} ; then l_{32} , l_{42} , l_{52} , \cdots , $l_{n-1, 2}$, $l_{n, 2}$ respectively; next j = 3, i = 1, 2, $3, \dots n-1$, n; we find r_{13} , r_{23} , r_{33} , then l_{43} , l_{53} , l_{63} , \cdots , $l_{n-1, 3}$, $l_{n, 3}$ respectively and so on. In case $r_{1i} = 0$, the procedure will, however, collapse.

The general formula for the product matrix S = FL, the results of which will constitute the first iteration step, is given as follows

$$s_{ij} = r_{ii} l_{ij} + \sum_{p=i+1}^{n} r_{ip} l_{pj}$$
[vii]

$$s_{ij} = r_{ij} + \sum_{p=l+1}^{n} r_{ip} l_{pj}$$
(viii)

In the computer the elements $[a_{ij}]$ are replaced by the elements $[s_{ij}]$, or in other words, no s_{ij} - storage is necessary. Therefore s_{ij} in (vii) and (viii) can be substituted by a_{ij} . This makes the program more automatic and more efficient and reduces the computing time. Moreover n^2 locations are preserved. It is important to note in this connection that storage often plays a very important part in this type of problems.

In the second iteration the transformed matrix $[a_{ij}]$ will be treated in the same way as it has been done for the first iteration with the original matrix $[a_{ij}]$. This process will cantinue till the continuously transformed matrix $[a_{ij}]$ becomes almost an upper triangular matrix or L matrix becomes nearly an identity matrix.

(b) Check. Trace check is performed.

(c) Memory requirements. About $n^2 + n(n+1)/2 + n(n+1)/2 + 90$ locations are necessary of which n^2 locations are required for the ratio A, n(n+1)/2 for L, n(n+1)/2 for R and about 90 words for the program.

(d) Computing time per iteration. (referring to formulae v, vi, vii, viii) It is about

$$\nu_{1} n (n-1)/2 + \nu_{2} \left\langle \left[\sum_{p=2}^{n} p (p-1)/2\right] + (n-1) (n-2)/2 + \sum_{p=0}^{n-1} \left[n (n+1)/2 - p\right] - n \right\rangle + \nu_{3} \left[n (n-1)/2 + (n-1) (n-2)/2\right] + \left\langle \sum_{p=2}^{n-1} p (p-1)/2 + \sum_{p=0}^{n-2} \left[n (n-1)/2 - p\right] \right\rangle \nu_{4} + \tau_{2} (n)$$

where the first 4 terms with ν 's deleted indicate number of divisions, multiplications, subtractions and additions respectively and $\tau_2(n)$ is the time needed by input and output units inclusive of that due to logical operations.

The difference between $\tau_1(n)$ and $\tau_2(n)$ is small, so that in the course of comparison these quantities can be neglected without affecting the process much.

*When n=5, *i.e.* for a matrix of order 5, computing time per iteration for method 1 is $70v'_1 + 54v'_3 + \tau_1(n)$ and for method 2 it is $96v'_1 + 60v'_3 + \tau_2(n)$. When n=7, computing time per iteration for method 1 is $203v'_1 + 161v'_3 + \tau_1(n)$ and for method 2, it is $:60v'_1 + 182v'_3 + \tau_2(n)$. When n=5, total storage required for method 1 is about 95 words while for method 2 it is 140 words. Therefore method 1 obviously saves on operational time and storage.

RESULTS

Calculations in all the examples are carried out in 8 dit floating point arithmetic and the results are retained correct up to 4 decimal places, unless otherwise stated. Zeros on the least significant side are avoided.

Example. 1 Matrix with double latent roots

A =	6	4	4	1	ĺ	1	5	0	0	0	$A \rightarrow$	15	5	5	1	
	4	6	1	4			5	5	0	0	2 passes,	0	5	0	3	12 passes,
	4	1	6	4		1	5	0	5	0	nethod 1,	0	0	5	3	method 2
	1	4	4	6	1	[1	3	3.	-1_	A = -375	0	0	0	-1_	

^{*}Y1=average time for one multiplication or one division

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V3 = average time for one addition or one subtraction.

Example, 2. Matrix with disorder of latent roots

The (2, 3)th element varies with the number of iterations. It becomes, 6173, .346, .1837, .0947, .0481, .0242, ¹.0121, .0059, .0010, -.0036, -.0249, -.1278, -.6407, -3.2043, -16.0218, -80.1091, -400.545 in the 1st, 2nd, 3rd, ..., 16th and 17th iterations respectively and does not converge.

10	- 6.7513	2	1			
0	1	0	01,.			•
 .0001	- 22 5028	5	1.5	passes,	mernoq	4
0	0	0	2			
-			-			

The latent roots are 10, 1, 5, 2. The differences between A_k 's in method 1 and method 2 are due to rounding errors only. Round-off errors are, however, more in method 2.

Example 3 Real matrix with one pair of complex roots

The exact roots are 6, $\pm i \sqrt{3}$

 $\rightarrow \begin{bmatrix} 6.0002 & -41108.1277 & 1 \\ .0001 & -82222.5661 & 2 \\ 5.7987 & -.338 \times 10^{10} & 82222.5665 \end{bmatrix}$ 11 passes, method 2

The 10th iteration step is $\begin{bmatrix} 6.0001 &$ **3.5 & 1 \\ -.0001 & -.0002 & 2 \\ .0004 & 7.8946 & .0002 \end{bmatrix}**

It can be seen that the last two diagonal terms in the 11th iteration are very large. This is evidently due to the fact that the last two diagonal elements of the 10th iteration step are very small and that they occur in denominators of (iv).

In both the methods the last two diagonal terms go on oscillating within the rounding error due to division as follows:

LABLE

No. of itera- tions	Method 1	Method 2
1	- 17, 18	- 17, 18
2	- ·9391, - ·2609	9391,2609
3	137-9167, -138-0001	137-9168, -138-0001
4	$\cdot 6143 \times 10^{-1}$, $\cdot 2076 \times 10^{-1}$	$\cdot 6143 \times 10^{-1}$, $\cdot 2076 \times 10^{-1}$
5	- 1732-5731, 1732-5800	- 17346·0023, 17346·0718
6	$5211 \times 10^{-2},1740 \times 10^{-2}$	$5234 \times 10^{-2},1724 \times 10^{-2}$
7	21463-6185, - 21463-6192	18328 -7695, - 18328-77
8	$\cdot 3662 \times 10^{-3}$, $\cdot 122 \times 10^{-3}$	$\cdot 4883 \times 10^{-3}, \cdot 2441 \times 10^{-3}$
9	46736-7895, - 46736-7895	- 64673·3895, 64673·3895
10	0, 0	2441×10^{-3} , -2441×10^{-3}
11	2-5582, -2-5582	- 82222-5661, 82222-5665
12	$\cdot 2739 \times 10^{-4}, - \cdot 3074 \times 10^{-4}$	0, $\cdot 2441 \times 10^{-3}$

The above tables also shows the effect of rounding errors due to divisions in both the methods. The rounding errors appear to play more important part in method 2.

If a real matrix possesses a pair of complex roots in its *i*-th and (i + 1) th rows, the elements in the *i*-th row and those in the *i*-th column below the diagonal¹³ will not converge in the normal way; the diagonal elements in the *i*-th and [i + 1] th row may go on oscillating as has been shown above.

Example 4. Matrix of order 4 with a pair of complex roots

 $\begin{array}{ccccc} A = & \begin{bmatrix} 4 - 5 & 0 & 3 \\ 0 & 4 - 3 - 5 \\ 5 - 3 & 4 & 0 \\ 3 & 0 & 5 & 4 \end{bmatrix}$ Exact roots; 12, 1 $\pm i\sqrt{5}$, 2

For real roots the first and last diagonal elements of A_k converge to 12 and 2 after 15th interation For complex roots the [2, 2]th, [2, 3]th, [3, 2]th and [3, 3]th elements do not appear to converge in the normal way. In the 7th iteration they become

 $B = \begin{bmatrix} .0072 & -5.1709 \\ 5.042 & 1.9336 \end{bmatrix}$

Now the roots μ_2 , μ_3 of B can be given by

 $\begin{vmatrix} .0072 - \mu & -5 \cdot 1709 \\ 5 \cdot 042 & 1 \cdot 9336 - \mu \end{vmatrix} = 0$

Therefore
$$\mu_{2,3} = .9704 \pm 15.0145$$

The divergence of μ_2 , μ_3 from the exact roots are due to rounding errors. In the case of single or multiple pairs of complex roots rounding errors play a very important part. These errors can be reduced by increasing the number of digits of the floating point arithmetic¹⁷.

Example 5: A symmetric matrix with distinct latent roots (convergence is slow for this particular matrix):

A =	$\begin{bmatrix} 2\\1\\-1\\2 \end{bmatrix}$	1 3 2 - 3	-1 2 1 -1	2 - 3 - 1 4	→ 7.4683 - 1.2335 - 4.1801 2	0 3.2753 - 4 4262 2.357	0 0 - 1.6405 9146	0 0 0 .8969	$\begin{vmatrix} 15 \text{ passes} \\ \text{method } 1, \\ A = -36 \end{vmatrix}$
	-			-	$\Rightarrow \begin{bmatrix} 7.4683 \\ -0.0003 \\ 0 \\ 0 \end{bmatrix}$	- 1.2335 3.2753 0 0	- 4 1801 - 4.4261 - 1.6405 0	2 2.3569 .9147 .897	15 passes, method 2

Example 6 : A defective matrix :

$$A = \begin{bmatrix} 6 & -3 & 4 & 1 \\ 4 & 2 & 4 & 0 \\ 4 & -2 & 3 & 1 \\ 4 & 2 & 3 & 1 \end{bmatrix} \rightarrow \begin{bmatrix} 5.5713 & -0.024 & 0 & 0 \\ 4.6833 & 4\,9008 & 0 & 0 \\ 2.5078 & -0.4179 & 0.825 & 0.0024 \\ 4 & 5.7137 & -1.5374 & 0.7029 \end{bmatrix}$$
 I4 passes,
method 1
$$\longrightarrow \begin{bmatrix} 5.5713 & -1.141 & 5.4818 & 1 \\ 0.0985 & 4\,9008 & -7.2257 & -2.0478 \\ 0 & 0 & -8.25 & 0.4358 \\ 0 & 0 & -0.0086 & 0.7029 \end{bmatrix}$$
 I4 passes,
method 2

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Example 7: Wilson's matrix :

$$A = \begin{bmatrix} 10 & 9 & 7 & 5 \\ 9 & 10 & 8 & 6 \\ 7 & 8 & 10 & 7 \\ 5 & 6 & 7 & 5 \end{bmatrix} \rightarrow \begin{bmatrix} 30.2887 & 0 & 0 & 0 \\ 42.27 & 3.3581 & 0 & 0 \\ 10.0199 & 1.0071 & .8431 & 0 \\ 5 & .7022 & .3168 & .0102 \end{bmatrix} \xrightarrow{\text{method } 1, \ A = 1} \\ \Rightarrow \begin{bmatrix} 30.2887 & 42.27 & 10.0199 & 5 \\ 0 & 3.8581 & 1.0071 & .7022 \\ 0 & 0 & .8431 & - .3168 \\ 0 & 0 & 0 & .0102 \end{bmatrix} \xrightarrow{\text{method } 2}$$

Example 8 : A stochastic matrix of order 4

A square matrix $A = (a_{ij})$ with non-negative elements is called stochascic²⁰ if

$$\sum_{j=1}^{n} a_{ij} = 1 \qquad i = 1, 2, 3, \dots, n-1, n$$

Such matrices are of great importance in the theory of probability.

<u>4</u> =	.31 .41 .21 .57	.32 .12 .24 .15	.33 .07 .25 .18	.04 .4 .3 .1	->-	1 .9335 4.885 .57	0 1555 1.951 2061	0 0368 0971 0119	0 0 0326	14 passes, method 1, A = .0028
					~~>	1 0 0	.5009 1555 .0812 0	.2608 8832 097 0	.04 .36 .0835 .0326	14 passes, method 2,

Example. 9. Hilbert's matrix

These matrices are typical examples of near singular matrices. Their singularity becomes more pronounced as their order is increased. In the following Hilbert's matrices of order 3, 4 and 5 have been considered, retaining every element correct up to 8 decimal places.

Hilbert's matrix of order 3 (determinant value = $\cdot 453 \times 10^{-8}$)

	1.4083	0	0				
~>	.8455	.1223	0	4	passes,	method	ĩ
	.3333	.0647	$.2687 \times 10^{-4}$				

Method 2 gives the same results (correct up to 4 decimal places) in the same number of passes as method 1.

Hilbert's matrix of order 4 (determinant value - $.1653 \times 10^{-6}$)

				an or here and a second s		
	1.5002	0	0	0		
~	1.1031	.1491	0	0	Courses muchad	
-	.7178	.1483	$.6738 \times 10^{-2}$	0	o passes, method	2
	.25	$.5746 \times 10^{-1}$	$.3918 \times 10^{-2}$	$.967 \times 10^{-4}$		
	distanting to the second se					

Method 2 gives the same result as method 1.

Hilbert's matrix of order 5 (determinant value = $.3743 \times 10^{-11}$)

According to both the methods the roots are 1.5671, .2085, .1141 $\times10^{-1}$.3059 $\times10^{-3}$, .3282 $\times10^{-5}$ in 7 passes.

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Example 10.

Roots found by method 1 and method 2 are 2, 2, 2. Roots obtained by 3.1 code (real code) of Eberlein¹⁶ are shown underscored in the matrix.

2.008	0 1.992	800. 0	0 7	10
800. – 1 0	0 .008	$\frac{2.008}{0}$	0 ' 1.991 '	10 passes.

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