COMPUTER METHODS IN APPLIED MECHANICS AND ENGINEERING 35 (1982) 255–269
NORTH-HOLLAND PUBLISHING COMPANY

RUTISHAUSER'S MODIFIED METHOD FOR COMPUTING THE EIGENVALUES OF SYMMETRIC MATRICES

Humberto Lima SORIANO*
COPPE, Federal University of Rio de Janeiro, Rio de Janeiro, Brazil

Received 27 August 1980
Revised manuscript received 1 March 1982

The purpose of this paper is to present a new procedure for the Rutishauser method (LR-method) of computing eigenvalues of symmetric matrices. This procedure is useful for real symmetric matrices with small band-widths. Shifts of origin are required for accelerating the process of convergence that may lead to indefinite matrices for which the classical approach is not applicable. The present approach demands only that the leading principal minors of the matrices operated have non-zero values. This paper compares this approach with the classical approach based on Cholesky factorizations and with the QR-method. The numerical results presented show the great effectiveness of the former.

0. Nomenclature

$\boldsymbol{A}_1$	a matrix with coefficients a_{ij}; the eigenvalues of this matrix are required;
$\boldsymbol{A}_k, \bar{\boldsymbol{A}}_k, \boldsymbol{A}_k^*, \bar{\boldsymbol{A}}_k^*$	matrices obtained at the kth iteration;
$\boldsymbol{L}_k, \bar{\boldsymbol{L}}_k$	lower-triangular matrices;
$\boldsymbol{R}, \boldsymbol{R}_k, \bar{\boldsymbol{R}}_1, \boldsymbol{U}_k^*, \bar{\boldsymbol{U}}_k^*$	upper-triangular matrices;
$\boldsymbol{U}_k, \bar{\boldsymbol{U}}_k$	upper-triangular matrices known as the Cholesky factors;
$\boldsymbol{D}, \boldsymbol{D}_k, \bar{\boldsymbol{D}}, \bar{\boldsymbol{D}}_k$	diagonal matrices;
d_i, d_k'	diagonal coefficients of $\boldsymbol{D}_k$ and $\boldsymbol{D}_{k-1}$, respectively;
$\boldsymbol{I}$	identity matrix;
λ_j	the jth eigenvalue of $\boldsymbol{A}_1$;
s_k	acceleration factor of the kth iteration;
$\boldsymbol{x}, \boldsymbol{y}$	vectors;
n	order of $\boldsymbol{A}_1$ or of the matrix which is being iterated at the kth iteration;
p	number of eigenvalues obtained before the kth iteration;
$f_l, \bar{f}$	semi-band-width of the lth row and average band-width of $\boldsymbol{A}_1$, respectively;
α	number of iterations for isolating an eigenvalue.

*Civil Engineer—D.Sc., Visiting Research Fellow of the Civil Engineering Department of the University of Southampton.

1. Introduction

In engineering, eigenvalue problems are commonly encountered. Various methods are available for the solution of these problems, each one having its own particular advantages and disadvantages.

A very precise method for real symmetric positive definite matrices is the Rutishauser method based on Cholesky factorizations. This method will be referred to as the LRC-method. The method is closely related to the Francis method, which is also known as the QR-method. In these methods shifts of origin are used for accelerating the process of convergence. If no shifts are used, two cycles of the LRC-method yield the same transformed matrix as one cycle of the QR-method. The QR-method enjoys a great numerical stability, but the requirement that the matrix be positive definite places strict limits on the shifts for the LRC-method. However, the QR-method demands orthogonal factorizations which require a volume of computation much larger than the simple Cholesky factorization. For indefinite matrices $\boldsymbol{A}$ with non-zero leading principal minors there is the factorization $\boldsymbol{A} = \boldsymbol{U}^{\mathrm{t}}\boldsymbol{E}\boldsymbol{U}$ which is intimately related to the classical Cholesky factorization. Here, $\boldsymbol{U}$ represents an upper-triangular matrix and $\boldsymbol{E}$ a diagonal matrix with coefficients equal to $+1$ or -1. However, this new factorization demands a larger number of additional multiplications than the classical Cholesky factorization [18]. Alternatively, the signs of $\boldsymbol{E}$ may be associated to $\boldsymbol{U}^{\mathrm{t}}$ leading to a triangular matrix which will not be the transpose of $\boldsymbol{U}$ [2]. For both cases the Rutishauser method yields a transformed non-symmetric matrix in each cycle of the process.

In this paper a new procedure for the Rutishauser method is presented for real symmetric matrices with non-zero leading principal minors. This new procedure will be referred to as the LRM-method. The transformed matrix at each cycle of the method is symmetric; this method eliminates both the matrix $\boldsymbol{E}$ and the square roots of the Cholesky factorization. It is as precise as the LRC-method and the QR-method, and much more stable than the LRC-method. In addition, it involves less computation than the QR-method.

2. Review of the classical approach of the Rutishauser method

The Rutishauser method known as the LR-method is based on the factorization of a square matrix $\boldsymbol{A}_1$ as follows

$$\boldsymbol{A}_1 = \boldsymbol{L}_1\boldsymbol{R}_1 . \tag{2.1}$$

$\boldsymbol{L}_1$ and $\boldsymbol{R}_1$ are a lower-triangular and an upper-triangular matrix, respectively. If the factorization (2.1) exists, and $\boldsymbol{A}_1$ is non-singular, this factorization is unique since the coefficients of the main diagonal of one of these triangular matrices are taken as being 1. $\boldsymbol{L}_1$ is usually chosen for this.

Using (2.1) the following sequence is defined

$$\boldsymbol{A}_k = \boldsymbol{L}_k\boldsymbol{R}_k , \tag{2.2.a}$$

$$\boldsymbol{A}_{k+1} = \boldsymbol{R}_k\boldsymbol{L}_k . \tag{2.2.b}$$

Assuming that

(i) $\boldsymbol{A}_1$ has unequal eigenvalues,

(ii) the leading principal minors of its modal matrix and of the inverse of the modal matrix are non null, then

$$\boldsymbol{A}_{k+1} = (\boldsymbol{R}_k \boldsymbol{R}_{k-1} \cdots \boldsymbol{R}_1)\boldsymbol{A}_1(\boldsymbol{R}_k \boldsymbol{R}_{k-1} \cdots \boldsymbol{R}_1)^{-1} \tag{2.3}$$

and

$$\lim_{k\to\infty} \boldsymbol{A}_k = \boldsymbol{R}\,. \tag{2.4}$$

$\boldsymbol{R}$ is an upper-triangular matrix. (2.3) shows that $\boldsymbol{A}_1$ and $\boldsymbol{A}_{k+1}$ are similar matrices. Therefore, the eigenvalues of $\boldsymbol{A}_1$ are the diagonal elements of $\boldsymbol{R}$.

For a real symmetric positive definite matrix $\boldsymbol{A}_1$ it is always possible to perform the Cholesky factorization

$$\boldsymbol{A}_1 = \boldsymbol{U}_1^{\mathrm{t}} \boldsymbol{U}_1\,. \tag{2.5}$$

$\boldsymbol{U}_1$ is a real upper-triangular matrix known as the Cholesky factor.

Using (2.5) the following sequence is defined

$$\boldsymbol{A}_k = \boldsymbol{U}_k^{\mathrm{t}} \boldsymbol{U}_k\,, \tag{2.6.a}$$

$$\boldsymbol{A}_{k+1} = \boldsymbol{U}_k \boldsymbol{U}_k^{\mathrm{t}}\,. \tag{2.6.b}$$

Thus, one has

$$\boldsymbol{A}_{k+1} = (\boldsymbol{U}_k \boldsymbol{U}_{k-1} \cdots \boldsymbol{U}_1)\boldsymbol{A}_1(\boldsymbol{U}_k \boldsymbol{U}_{k-1} \cdots \boldsymbol{U}_1)^{-1} \tag{2.7}$$

and

$$\lim_{k\to\infty} \boldsymbol{A}_k = \boldsymbol{D} \tag{2.8}$$

where $\boldsymbol{D}$ is a diagonal matrix. Therefore, the eigenvalues of $\boldsymbol{A}_1$ are equal to the diagonal coefficients of $\boldsymbol{D}$. This is a very precise method for obtaining eigenvalues. There are no restrictions on convergence for sequence (2.6), and the spectral norm of $\boldsymbol{A}_k$ is equal to the spectral norm of $\boldsymbol{A}_1$. This method is here called the LRC-method.

To improve the rate of convergence of this method it is necessary to make a shift of origin s_k in each iteration k. Thus, one obtains

$$\boldsymbol{A}_k' = (\boldsymbol{A}_k - s_k \boldsymbol{I})\,. \tag{2.9}$$

The quantity s_k is here called the acceleration factor. This factor must be almost equal to, and smaller than, the eigenvalue λ_j which is being obtained in the kth iteration. If s_k is greater than λ_j, then (2.9) gives an indefinite matrix and the factorization (2.6a) becomes unstable for real numbers. A judicious choice of s_k is not easy, and the numerical stability of the method is difficult to obtain. The new procedure presented below reduces the risk that unsuitable values of s_k will be chosen.

3. The LRM-method

Considering a real symmetric matrix with non-zero leading principal minors, one has the factorization

$$\boldsymbol{A}_1 = (\boldsymbol{L}_1\boldsymbol{D}_1^{1/2})(\boldsymbol{D}_1^{1/2}\boldsymbol{L}_1^{\mathrm{t}}) = \boldsymbol{U}_1^{\mathrm{t}}\boldsymbol{U}_1 \,. \tag{3.1}$$

In this last equation $\boldsymbol{L}_1$ and $\boldsymbol{U}_1$ are matrices as defined previously, and $\boldsymbol{D}_1$ is a diagonal matrix. The coefficients of $\boldsymbol{D}_1$ may be positive or negative allowing complex numbers in matrices $\boldsymbol{D}_1^{1/2}$ and $\boldsymbol{U}_1$.

Using (3.1) one can write

$$\boldsymbol{A}_2 = \boldsymbol{U}_1\boldsymbol{U}_1^{\mathrm{t}} = \boldsymbol{D}_1^{1/2}\boldsymbol{L}_1^{\mathrm{t}}\boldsymbol{L}_1\boldsymbol{D}_1^{1/2} \,. \tag{3.2}$$

Defining

$$\boldsymbol{A}_2^* = \boldsymbol{L}_1^{\mathrm{t}}\boldsymbol{L}_1 = \boldsymbol{L}_2\boldsymbol{D}_2\boldsymbol{L}_2^{\mathrm{t}} \,, \tag{3.3}$$

(3.2) gives

$$\boldsymbol{A}_2 = \boldsymbol{D}_1^{1/2}\boldsymbol{A}_2^*\boldsymbol{D}_1^{1/2} = \boldsymbol{D}_1^{1/2}\boldsymbol{L}_2\boldsymbol{D}_2^{1/2}\boldsymbol{D}_2^{1/2}\boldsymbol{L}_2^{\mathrm{t}}\boldsymbol{D}_1^{1/2} \,, \tag{3.4}$$

thus

$$\boldsymbol{A}_2 = \boldsymbol{U}_2^{\mathrm{t}}\boldsymbol{U}_2 \tag{3.5}$$

where

$$\boldsymbol{U}_2 = \boldsymbol{D}_2^{1/2}\boldsymbol{L}_2^{\mathrm{t}}\boldsymbol{D}_1^{1/2} \,. \tag{3.6}$$

Since the Cholesky factorization is unique for a positive definite matrix $\boldsymbol{A}_1$, the matrix $\boldsymbol{A}_2$ obtained by (3.5) is equal to that obtained by (2.6a) when k is equal to 2. Therefore, the results of (2.6) can be obtained in a different way as shown below. Defining

$$\boldsymbol{A}_k^* = \boldsymbol{L}_{k-1}^{\mathrm{t}}\boldsymbol{D}_{k-2}\boldsymbol{L}_{k-1} \,, \tag{3.7}$$

one can write the sequence

$$\boldsymbol{A}_k = \boldsymbol{D}_{k-1}^{1/2}\boldsymbol{A}_k^*\boldsymbol{D}_{k-1}^{1/2} \,, \tag{3.8.a}$$

$$\boldsymbol{A}_k = \boldsymbol{D}_{k-1}^{1/2}\boldsymbol{L}_k\boldsymbol{D}_k^{1/2}\boldsymbol{D}_k^{1/2}\boldsymbol{L}_k^{\mathrm{t}}\boldsymbol{D}_{k-1}^{1/2} \,, \tag{3.8.b}$$

$$\boldsymbol{A}_{k+1} = \boldsymbol{D}_k^{1/2}(\boldsymbol{L}_k^{\mathrm{t}}\boldsymbol{D}_{k-1}\boldsymbol{L}_k)\boldsymbol{D}_k^{1/2} \,, \tag{3.8.c}$$

$$\boldsymbol{A}_{k+1} = \boldsymbol{D}_k^{1/2}\boldsymbol{A}_{k+1}^*\boldsymbol{D}_k^{1/2} \,. \tag{3.8.d}$$

In [1] it is shown that the values of coefficients in this last sequence do not increase as the sequence is performed.

Using (2.8) and (3.8.d), one has

$$\lim_{k\to\infty} \boldsymbol{D}_k^{1/2}\boldsymbol{A}_{k+1}^*\boldsymbol{D}_k^{1/2} = \boldsymbol{D} \tag{3.9}$$

where the diagonal matrix $\boldsymbol{D}$ contains the eigenvalues of $\boldsymbol{A}_1$. Since $\boldsymbol{D}$ is a diagonal matrix, its coefficients in the limit can be obtained by multiplying the diagonal coefficients of $\boldsymbol{A}^*_{k+1}$ by the corresponding elements of $\boldsymbol{D}_k$. Consequently, the whole process is free of square roots and complex numbers, because one does not need to compute $\boldsymbol{D}_k^{1/2}$. In this process the real symmetric matrix $\boldsymbol{A}_1$ and the intermediate matrix $\boldsymbol{A}^*_k$ need only to have non-zero leading principal minors.

For accelerating the process, using (3.8.a) one obtains

$$\boldsymbol{A}_k - s_k\boldsymbol{I} = \boldsymbol{D}_{k-1}^{1/2}\boldsymbol{A}^*_k\boldsymbol{D}_{k-1}^{1/2} - s_k\boldsymbol{I}$$

and

$$\boldsymbol{A}_k - s_k\boldsymbol{I} = \boldsymbol{D}_{k-1}^{1/2}(\boldsymbol{A}^*_k - s_k\boldsymbol{D}_{k-1}^{-1})\boldsymbol{D}_{k-1}^{1/2}\,. \tag{3.10}$$

This last equation shows that to consider the acceleration factor at the kth iteration, one needs to subtract from each coefficient of the main diagonal of $\boldsymbol{A}^*_k$ the quantity s_k divided by the corresponding coefficient of the diagonal matrix $\boldsymbol{D}_{k-1}$. Factorizing the bracketed term in (3.10), one obtains

$$\boldsymbol{A}_k - s_k\boldsymbol{I} = (\boldsymbol{D}_{k-1}^{1/2}\boldsymbol{L}_k\boldsymbol{D}_k^{1/2})(\boldsymbol{D}_k^{1/2}\boldsymbol{L}_k^{\mathrm{t}}\boldsymbol{D}_{k-1}^{1/2}) \tag{3.11}$$

and

$$\boldsymbol{A}_{k+1} = \boldsymbol{D}_k^{1/2}(\boldsymbol{L}_k^{\mathrm{t}}\boldsymbol{D}_{k-1}\boldsymbol{L}_k)\boldsymbol{D}_k^{1/2} + s_k\boldsymbol{I}\,. \tag{3.12}$$

Substituting (3.7) into (3.12), one has

$$\boldsymbol{A}_{k+1} = \boldsymbol{D}_k^{1/2}\boldsymbol{A}^*_{k+1}\boldsymbol{D}_k^{1/2} + s_k\boldsymbol{I}\,. \tag{3.13}$$

(3.11) yields

$$\boldsymbol{D}_{k-1}^{1/2}\boldsymbol{L}_k\boldsymbol{D}_k^{1/2} = (\boldsymbol{A}_k - s_k\boldsymbol{I})(\boldsymbol{D}_{k-1}^{-1/2}\boldsymbol{L}_k^{-\mathrm{t}}\boldsymbol{D}_k^{-1/2})\,. \tag{3.14}$$

Then, using (3.12) and (3.14) one can write

$$\boldsymbol{A}_{k+1} = (\boldsymbol{D}_k^{1/2}\boldsymbol{L}_k^{\mathrm{t}}\boldsymbol{D}_{k-1}^{1/2})(\boldsymbol{A}_k - s_k\boldsymbol{I})(\boldsymbol{D}_{k-1}^{-1/2}\boldsymbol{L}_k^{-\mathrm{t}}\boldsymbol{D}_k^{-1/2}) + s_k\boldsymbol{I}$$

and

$$\boldsymbol{A}_{k+1} = (\boldsymbol{D}_k^{1/2}\boldsymbol{L}_k^{\mathrm{t}}\boldsymbol{D}_{k-1}^{1/2})\boldsymbol{A}_k(\boldsymbol{D}_k^{1/2}\boldsymbol{L}_k^{\mathrm{t}}\boldsymbol{D}_{k-1}^{1/2})^{-1}\,. \tag{3.15}$$

This last equation shows that $\boldsymbol{A}_k$ and $\boldsymbol{A}_{k+1}$ are similar matrices and therefore have the same eigenvalues. (3.13) shows that the factor s_k is restored in the $(k+1)$th iteration. Alternatively, one can proceed as follows:

$$\begin{aligned}
\boldsymbol{A}_{k+1} &= (\boldsymbol{D}_k^{1/2}\boldsymbol{L}_k^{\mathrm{t}}\boldsymbol{D}_{k-1}^{1/2})(\boldsymbol{A}_k - s_k\boldsymbol{I})(\boldsymbol{D}_k^{-1/2}\boldsymbol{L}_k^{-\mathrm{t}}\boldsymbol{D}_k^{-1/2})\,,\\
\boldsymbol{A}_{k+1} &= (\boldsymbol{D}_k^{1/2}\boldsymbol{L}_k^{\mathrm{t}}\boldsymbol{D}_{k-1}^{1/2})\boldsymbol{A}_k(\boldsymbol{D}_k^{1/2}\boldsymbol{L}_k^{\mathrm{t}}\boldsymbol{D}_{k-1}^{1/2})^{-1} - s_k\boldsymbol{I}\,,\\
\boldsymbol{A}_{k+1} &= (\boldsymbol{D}_k^{1/2}\boldsymbol{L}_k^{\mathrm{t}}\boldsymbol{D}_{k-1}^{1/2})(\boldsymbol{D}_{k-1}^{1/2}\boldsymbol{L}_{k-1}^{\mathrm{t}}\boldsymbol{D}_{k-2}^{1/2})\boldsymbol{A}_{k-1}(\boldsymbol{D}_{k-1}^{1/2}\boldsymbol{L}_{k-1}^{\mathrm{t}}\boldsymbol{D}_{k-2}^{1/2})^{-1}(\boldsymbol{D}_k^{1/2}\boldsymbol{L}_k^{\mathrm{t}}\boldsymbol{D}_{k-1}^{1/2})^{-1}\\
&\quad - (s_k + s_{k-1})\boldsymbol{I}\,.
\end{aligned} \tag{3.16}$$

Pursuing the development of this last equation, one obtains

$$\boldsymbol{A}_{k+1} = \boldsymbol{U}_k^* \boldsymbol{A}_1 \boldsymbol{U}_k^{*-1} - \sum_{j=1}^{k} s_j \boldsymbol{I} \tag{3.17}$$

where

$$\boldsymbol{U}_k^{*t} = \prod_{j=1}^{k} (\boldsymbol{D}_j^{1/2} \boldsymbol{L}_j^t \boldsymbol{D}_{j-1}^{1/2})^t \tag{3.18}$$

for $\boldsymbol{D}_0 = \boldsymbol{I}$. (3.17) shows that the eigenvalues of $\boldsymbol{A}_{k+1}$ are different from those of $\boldsymbol{A}_1$ by the amount $(\Sigma_{j=1}^{k} s_j \boldsymbol{I})$ which must be restored at the end of the converging process. Thus,

$$\boldsymbol{D} = \lim_{k \to \infty} \boldsymbol{D}_k^{1/2} \boldsymbol{A}_{k+1}^* \boldsymbol{D}_k^{1/2} + \sum_{j=1}^{k} s_j \boldsymbol{I}. \tag{3.19}$$

This last procedure is much simpler than the previous one, in which the acceleration factor is restored at each iteration. In the kth iteration this factor must be near to the eigenvalue λ_j which is being obtained and a value for this factor may be computed from the results of the $(k-1)$th iteration. It can be proved that the convergence towards the eigenvalues occurs sequentially, according to their magnitudes, on the main diagonal of $\boldsymbol{A}_k$, as shown in Fig. 1. When a specific eigenvalue is reached, its corresponding row and column no longer need to be operated.

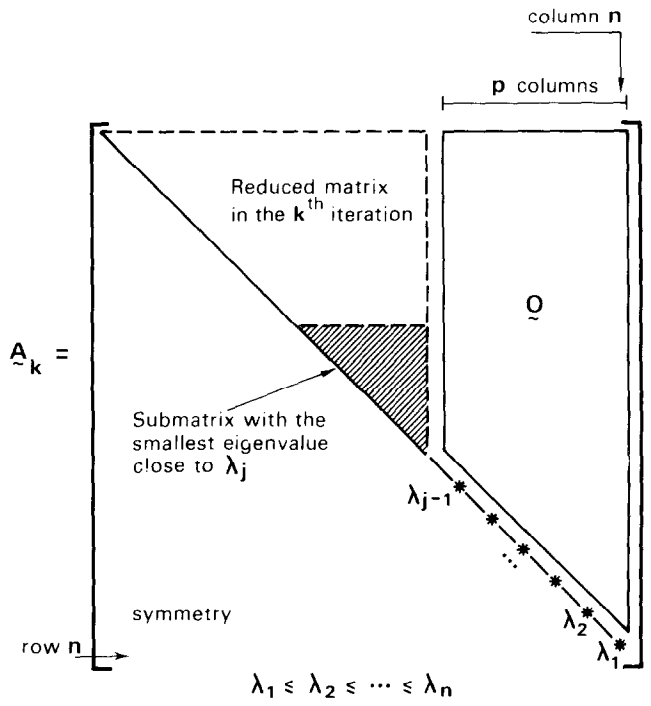


Fig. 1. Principal submatrix giving the acceleration factor for a particular eigenvalue λ_j.

Defining

$$\boldsymbol{U}_k = \boldsymbol{D}_{k-2}^{1/2}\boldsymbol{L}_{k-1}\boldsymbol{D}_{k-1}^{1/2} \tag{3.20}$$

using (3.7) and (3.8.a) one can write

$$\boldsymbol{A}_{k+1} = \boldsymbol{U}_k^{\mathrm{t}}\boldsymbol{U}_k\,. \tag{3.21}$$

Designating n the order of matrix $\boldsymbol{A}_1$ and p the number of the eigenvalues obtained before the kth iteration, it is possible to prove that the coefficients of $\boldsymbol{U}_k$ belonging to the first $(n-p)$ rows and the last p columns converge towards zero. Thus, a viable suggestion for the factor s_k is the smallest eigenvalue of a principal submatrix as indicated in Fig. 1. [1] develops expressions to give explicitly the eigenvalues of that submatrix for order 2 and 3. The same LRM-method may be used to compute the smallest eigenvalue of submatrices of order larger than 3. However, for the classical approach of the LR-method the use of order 2 is more common. It is important to point out that the adoption of acceleration factors may alter the natural order of convergence of the eigenvalues. For the numerical results presented in this paper, the LRM-method showed itself stable for the chosen acceleration factors; the Burroughs 6700 computer was used. It is important to note that in the case of a mistaken choice of a particular acceleration factor, it is possible to resume the corresponding iteration using a different value. Alternatively, for an unsuitable choice of s_k it is possible to introduce interchanges in the LRM-method. [2, p. 498] shows the use of interchanges for the LR-method; similar interchanges can be used for the LRM-method. However, on modern computers, very large and very small numbers can be represented. Therefore the probability of an unsuitable choice has decreased and in the case of a bad choice of s_k, the most simple remedy is to adopt a different value.

4. The LRM-method in reverse order

The matrix $\boldsymbol{A}_1$ of (3.1) can also be factorized as follows:

$$\boldsymbol{A}_1 = (\bar{\boldsymbol{L}}_1^{\mathrm{t}}\bar{\boldsymbol{D}}_1^{1/2})(\bar{\boldsymbol{D}}_1^{1/2}\bar{\boldsymbol{L}}_1) = \bar{\boldsymbol{U}}_1\bar{\boldsymbol{U}}_1^{\mathrm{t}}\,. \tag{4.1}$$

$\bar{\boldsymbol{L}}_1$ and $\bar{\boldsymbol{D}}_1$ are a lower-triangular matrix in which its diagonal coefficients are equal to 1 and a diagonal matrix, respectively. $\bar{\boldsymbol{U}}_1$ is an upper-triangular matrix. The coefficients of $\bar{\boldsymbol{D}}_1$ may be positive or negative allowing complex numbers in matrices $\bar{\boldsymbol{D}}_1^{1/2}$ and $\bar{\boldsymbol{U}}_1$.

If one adopts the notation

$$\bar{\boldsymbol{R}}_1 = \bar{\boldsymbol{L}}_1^{\mathrm{t}}\bar{\boldsymbol{D}}_1 \tag{4.2}$$

one obtains

$$\bar{\boldsymbol{R}}_1 = \bar{\boldsymbol{U}}_1\bar{\boldsymbol{D}}_1^{1/2} \tag{4.3}$$

and

$$\bar{\boldsymbol{U}}_1 = \bar{\boldsymbol{R}}_1 \bar{\boldsymbol{D}}_1^{-1/2} . \tag{4.4}$$

Taking the set of linear algebraic equations

$$\boldsymbol{A}_1 \boldsymbol{x} = \boldsymbol{y} \tag{4.5}$$

and considering (4.2) and (4.1), one has

$$\bar{\boldsymbol{R}}_1^t \boldsymbol{x} = \bar{\boldsymbol{L}}_1^{-t} \boldsymbol{y} . \tag{4.6}$$

This last equation may be obtained from the system (4.5) by a backward substitution. (4.4) shows that the Cholesky factor $\bar{\boldsymbol{U}}_1$ may be obtained by dividing each column of the triangular matrix $\bar{\boldsymbol{R}}_1$ by the square root of the corresponding diagonal coefficient of $\bar{\boldsymbol{R}}_1$.

Using (4.1) in the same way as for (2.2), one has the sequence

$$\bar{\boldsymbol{A}}_k = \bar{\boldsymbol{U}}_k \bar{\boldsymbol{U}}_k^t , \tag{4.7.a}$$

$$\bar{\boldsymbol{A}}_{k+1} = \bar{\boldsymbol{U}}_k^t \bar{\boldsymbol{U}}_k \tag{4.7.b}$$

for $\bar{\boldsymbol{A}}_1 = \boldsymbol{A}_1$. This last sequence gives in the limit a diagonal matrix $\bar{\boldsymbol{D}}$, the coefficients of which are equal to the eigenvalues of $\boldsymbol{A}_1$ sequentially according to their magnitudes. These eigenvalues are partitioned on the reverse of the order represented in Fig. 1.

Defining

$$\bar{\boldsymbol{A}}_k^* = \bar{\boldsymbol{L}}_{k-1} \bar{\boldsymbol{D}}_{k-2} \bar{\boldsymbol{L}}_{k-1}^t \tag{4.8}$$

in the same way as for (3.8), one can write the sequence

$$\bar{\boldsymbol{A}}_k = \bar{\boldsymbol{D}}_{k-1}^{1/2} \bar{\boldsymbol{A}}_k^* \bar{\boldsymbol{D}}_{k-1}^{1/2} , \tag{4.9.a}$$

$$\bar{\boldsymbol{A}}_k = \bar{\boldsymbol{D}}_{k-1}^{1/2} \bar{\boldsymbol{L}}_k^t \bar{\boldsymbol{D}}_k^{1/2} \bar{\boldsymbol{D}}_k^{1/2} \bar{\boldsymbol{L}}_k \bar{\boldsymbol{D}}_{k-1}^{1/2} , \tag{4.9.b}$$

$$\bar{\boldsymbol{A}}_{k+1} = \bar{\boldsymbol{D}}_k^{1/2} (\bar{\boldsymbol{L}}_k \bar{\boldsymbol{D}}_{k-1} \bar{\boldsymbol{L}}_k^t) \bar{\boldsymbol{D}}_k^{1/2} , \tag{4.9.c}$$

$$\bar{\boldsymbol{A}}_{k+1} = \bar{\boldsymbol{D}}_k^{1/2} \bar{\boldsymbol{A}}_{k+1}^* \bar{\boldsymbol{D}}_k^{1/2} . \tag{4.9.d}$$

Taking

$$\bar{\boldsymbol{U}}_k^* = \sum_{j=1}^{k} \bar{\boldsymbol{D}}_{j-1}^{1/2} \bar{\boldsymbol{L}}_j^t \bar{\boldsymbol{D}}_j^{1/2} \tag{4.10}$$

for $\bar{\boldsymbol{D}}_0 = \boldsymbol{I}$, one obtains

$$\bar{\boldsymbol{A}}_{k+1} = \bar{\boldsymbol{U}}_k^{*-1} \boldsymbol{A}_1 \bar{\boldsymbol{U}}_k^* \tag{4.11}$$

and

$$\lim_{k \to \infty} \boldsymbol{D}_k^{1/2} \bar{\boldsymbol{A}}_{k+1}^* \bar{\boldsymbol{D}}_k^{1/2} = \bar{\boldsymbol{D}} . \tag{4.12}$$

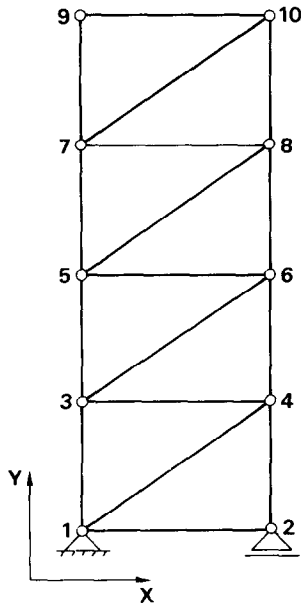
As in the case of (3.9) the eigenvalues of $\boldsymbol{A}_1$ can be obtained free of square roots and complex numbers. Acceleration factors can be adopted as in (3.19).

5. LRM algorithms

In this item, algorithms for band matrices when using sequence (3.8) are presented. The coefficients of $\boldsymbol{L}_k^t$ are given the same names as those of $\boldsymbol{A}_1$, namely a_{ij}. The diagonal coefficients of $\boldsymbol{D}_k$ are named d_i. f_l is the semi-band width of the lth row of $\boldsymbol{A}_1$ as represented in Fig. 2. Thus, $a_{lj} = 0$ for $j > l + f_l$.

Defining p as the number of eigenvalues obtained before the kth iteration and d_i as the ith coefficient of the diagonal matrix $\boldsymbol{D}_k$ one has

→ For $l = 1 \rightarrow (n - 1 - p)$
  → For $i = (l + 1) \rightarrow (l + f_l - 1) \leqslant (n - p)$
    $d_i = a_{li}$
  → For $i = (l + 1) \rightarrow (l + f_l - 1) \leqslant (n - p)$
    $a_{li} = a_{li}/a_{ll}$
    → For $j = i \rightarrow (l + f_l - 1) \leqslant (n - p)$
      $a_{ij} = a_{ij} - d_j a_{li}$
  $d_l = a_{ll}$
  $a_{ll} = 1$
$d_{n-p} = a_{n-p,n-p}$
$a_{n-p,n-p} = 1$



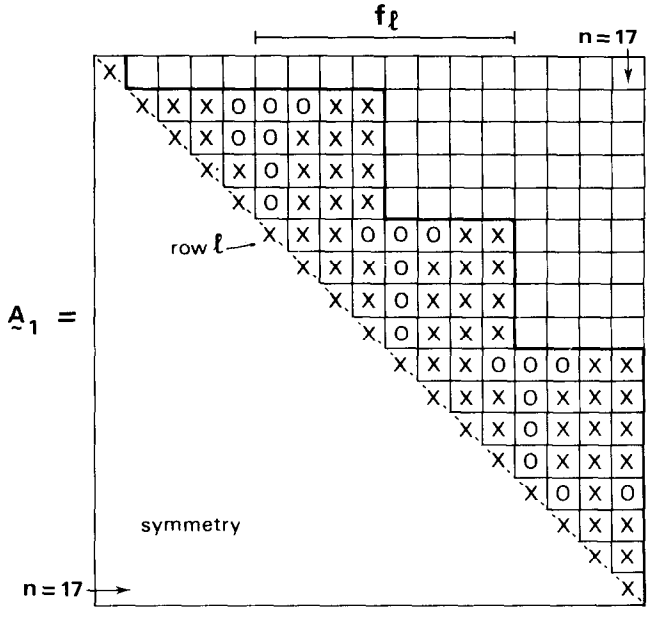


Fig. 2. Coefficients operated in sequence (3.8) for the band stiffness matrix of the plane truss shown.

The zero-coefficients represented in the variable band-widths of Fig. 2 were considered because they may differ from zero during the sequence (3.8). After obtaining $\boldsymbol{L}_k^t$ and $\boldsymbol{D}_k$, one can compute the upper-part of $\boldsymbol{A}_{k+1}^*$ by the following algorithm:

```
For i = 1 → (n − p)
    For k = i → (i + f_i − 1) ≤ (n − p)
        g_k = a_ik d'_k
    For j = i → (i + f_i − 1) ≤ (n − p)
        h = 0
        For k = j → (j + f_i − 1) ≤ (n − p)
            h = h + g_k a_jk
        a_ij = h
```

In this algorithm g_k represents the coefficients of an auxiliary vector; h is an auxiliary variable, and d_k' represents the coefficients of the diagonal matrix $\boldsymbol{D}_{k-1}$.

The verification of the convergence of eigenvalues in this method is done as usual and at the end of the kth iteration the approximate eigenvalues are obtained as follows:

```
For i = 1 → (n − p)
    λ_i = a_ii d_i + s
```

where $s = \Sigma_{j=1}^{k} s_j$.

6. Number of operations in the LRM-method for band matrices

Considering that in matrix operations an arithmetical multiplication or division is most of the time accompanied by an addition or subtraction, only the former two arithmetical operations will be considered here.

Defining the average band-width of the matrix represented in Fig. 2 by

$$\bar{f} = \sum_{l=1}^{n} f_l/n \tag{6.1}$$

each iteration of sequence (3.8) has a number of operations as given in Table 1.

Table 1

$\boldsymbol{L}_k^t$	$\frac{1}{2}n(\bar{f}^2+\bar{f}-2)-\frac{1}{3}\bar{f}(\bar{f}^2-1)$
$\boldsymbol{L}_k^t\boldsymbol{D}_{k-1}$	$\frac{1}{2}(2n\bar{f}-\bar{f}^2+\bar{f})$
$\boldsymbol{A}_{k+1}^*$	$\frac{1}{2}(n+n\bar{f}^2)$
Total number	$n\bar{f}^2+\frac{1}{2}(n(3\bar{f}-1)+\bar{f}(1-\bar{f}))-\frac{1}{3}\bar{f}(\bar{f}^2-1)$

The number of iterations needed in order to obtain each eigenvalue is a function of the acceleration factors used and the nature of A_1. If α represents this number, approximately $(\alpha n\bar{f}^2 + 1.5\alpha n\bar{f})$ operations are necessary to obtain each eigenvalue. Here, n represents the order of the reduced matrix in the kth iteration after the elimination of the rows and columns corresponding to the eigenvalues obtained before this iteration. In the examples presented in Section 7.2 below, 1.5 iterations were necessary per eigenvalue. Thus, the application of the present method is only advisable in the case of small band-widths. For a tri-diagonal matrix, the factorization of matrix A_k^* and the computation of the bracketed term of (3.8.c) can be obtained in only one loop allowing a very efficient algorithm, as shown by [1].

7. Numerical results

The following methods, for computing eigenvalues, are compared here:

(i) LRC—the LR-method with Cholesky factorizations.
(ii) QRH—the QR-method with Householder factorizations.
(iii) QRG—the QR-method with Gram–Schmidt factorizations.
(iv) LRM—the present approach represented by (3.8).

The symbol /DP is added to the above abbreviations to indicate that the whole process was carried out in double precision. The symbol /NF is used to indicate that the first iteration of sequence (3.8) was performed using the Cholesky factor obtained by the natural factor formulation. As discussed by [14, 15, 16, 17] this formulation leads to Cholesky factors with greater accuracy than the classical approach of the stiffness method.

7.1. Comparative tests using Hilbert matrices

Hilbert matrices are real symmetric positive definite matrices [8] and for the single precision of the Burroughs 6700 computer, their analysis begin to become critical, on account of rounding errors, for matrices of order 9 and above. Table 2 presents a comparison of eigenvalues of that matrix for order 9, for which the spectral conditioning number is 0.49×10^{12}. This conditioning number is defined as the ratio of the larger eigenvalue to the lower eigenvalue of the matrix. The single and double precision results are given for the eigenvalues λ_1 to λ_4. It can be seen that the results agree with increasing precision as the eigenvalues increase. The last digit of each single precision result is the first digit which differs from the correct result.

Table 2
Hilbert matrix of order 9

	$\lambda_1/10^{-11}$	$\lambda_2/10^{-9}$	$\lambda_3/10^{-7}$	$\lambda_4/10^{-5}$
LRM/DP QRH/DP QRG/DP	0.348128358	0.646005460	0.538562628	0.267301397
QRG	0.35	0.6461	0.538563	0.267301393
QRH	0.35	0.6458	0.538560	0.2673014
LRM	0.32	0.6459	0.538563	0.26730136
LRC	0.33	0.64607	0.538563	0.2673014

Table 3
Hilbert matrix of order 10

	λ_1	$\lambda_2/10^{-10}$	$\lambda_3/10^{-8}$	$\lambda_4/10^{-6}$
LRM/DP QRG/DP QRH/DP	—	0.226992089	0.214740814	0.122896797
QRG	—	0.227	0.21473	0.1228966
QRH	—	0.23	0.21477	0.1228969
LRM	—	0.228	0.214741	0.1228969

Table 2 shows that all the methods considered gave a similar precision. The lower precision of the first eigenvalues is due to the initial truncation of $\boldsymbol{A}_1$ when this matrix is represented on the computer.

Table 3 presents a comparison of the first four eigenvalues of the Hilbert matrix of order 10, which has spectral conditioning number 1.6×10^{13}. It was not possible to compute the first eigenvalue using any of those methods. The remaining eigenvalues were computed using all the methods considered but LRC. This exception is due to the fact that the initial truncation of $\boldsymbol{A}_1$ leads to an indefinite matrix for which LRC is unstable in respect of real numbers.

Table 3 shows that the LRM-method remains stable and precise, as does the QR-method with Householder or Gram–Schmidt factorizations.

7.2. Comparative tests for ill-conditioned trusses

This series of results refers to the cantilever truss represented in Fig. 3. This model was adopted by [15] in a comparative study between the classical approach of the stiffness method and the natural factor approach.

In the truss of Fig. 3, k_i represents the stiffness of the ith structural element. This truss was designed so that in the first example, all the elements have the same stiffness; in the other examples the relation between the stiffness of element 8 and the other elements is successively

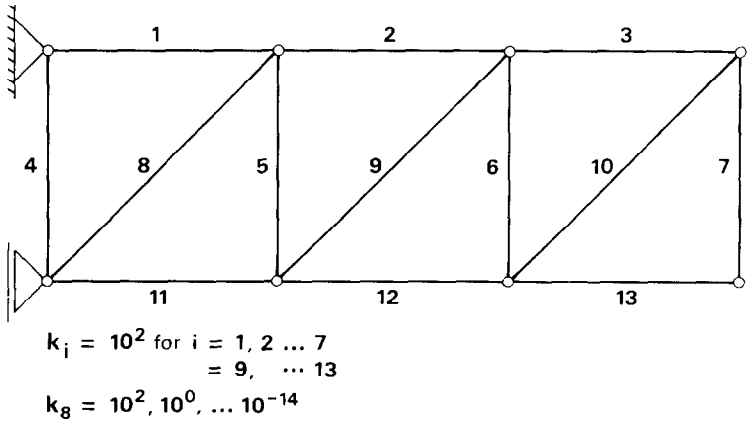


Fig. 3. Cantilever truss adopted by [15].

divided by 100. Discrete nodal masses equal to 1 were assumed, so that the dynamic matrix coincides with the stiffness matrix.

Tables 4–7 present the spectral conditioning numbers calculated by the methods considered. The results given by LRM/NF/DP were used as a reference. Tables 4–7 show that the LRM-method again led to results similar to those obtained by QRH and QRG respectively. Comparing the results of LRM/NF with those of the LRM-method, it becomes evident that it is the magnitude of the initial truncation of A_1 that is most responsible for the imprecision of the results. Besides this, the rounding errors diminish after the first iteration of the LRM sequence, because A_k^* tends towards a dominant diagonal matrix.

All the eigenvalues were computed by the QR and the LRM respectively, with the same convergence test and the same acceleration factors. The lowest eigenvalue of the submatrix of order 3, as represented in Fig. 1, was adopted as the acceleration factor. The QR-method required 17 iterations and the LRM-method 24. It is important to note that the number of iterations in the LRM-method was about 1.5 times the number in the QR-method, and not twice the number, as would happen if acceleration factors were not used. Acceleration factors were not considered for LRC, which required 248 iterations.

Table 4
Spectral conditioning numbers for the cantilever truss represented in Fig. 3 for the LRM/NF/DP- and LRM/DP-method

Example	k_i/k_8	LRM/NF/DP		LRM/DP	
1	10^0	0.372327286	10^3	0.372327286	10^3
2	10^2	0.554506193	10^4	0.554506193	10^4
3	10^4	0.529809338	10^6	0.529809338	10^6
4	10^6	0.529565891	10^8	0.529565891	10^8
5	10^8	0.529563456	10^{10}	0.529563456	10^{10}
6	10^{10}	0.529563432	10^{12}	0.529563432	10^{12}
7	10^{12}	0.529563432	10^{14}	0.529563432	10^{14}
8	10^{14}	0.529563432	10^{16}	0.529563432	10^{16}
9	10^{16}	0.529563432	10^{18}	0.529563	10^{18}

Table 5
Spectral conditioning numbers for the cantilever truss represented in Fig. 3 for the QRG/DP- and QRH/DP- and LRC/DP-method

Example	QRG/DP and QRH/DP		LRC/DP	
1	0.372327286	10^3	0.372327286	10^3
2	0.554506193	10^4	0.554506193	10^4
3	0.529809338	10^6	0.529809338	10^6
4	0.529565891	10^8	0.529565891	10^8
5	0.529563456	10^{10}	0.529563456	10^{10}
6	0.529563432	10^{12}	0.529563432	10^{12}
7	0.529563432	10^{14}	0.52956343	10^{14}
8	0.5295634	10^{16}	0.529563	10^{16}
9	0.52956	10^{18}	0.5295	10^{18}

Table 6
Spectral conditioning numbers for the cantilever truss represented in Fig. 3 for the LRM/NF- and LRM-method

Example	LRM/NF		LRM	
1	0.372327286	10^3	0.372327286	10^3
2	0.554506193	10^4	0.554506193	10^4
3	0.529809338	10^6	0.5298093	10^6
4	0.52956589	10^8	0.5295	10^8
5	0.52956345	10^{10}	0.529	10^{10}
6	0.529563	10^{12}	0.5	10^{12}
7	0.52956	10^{14}	—	
8	0.529	10^{16}	—	
9	0.5	10^{18}	—	

Table 7
Spectral conditioning numbers for the cantilever truss represented in Fig. 3 for the QRH- and QRG-method

Example	QRH		QRG	
1	0.372327286	10^3	0.372327286	10^3
2	0.5545061	10^4	0.55450619	10^4
3	0.52980933	10^6	0.529809	10^6
4	0.5295	10^8	0.5295	10^8
5	0.52	10^{10}	0.5	10^{10}
6	—		—	

8. Conclusions

The examples given illustrate that for the same initial truncation of $\boldsymbol{A}_1$ the methods considered give very close results. The present approach, the LRM-method, is much more stable than the classical approach of the LR-method using Cholesky factorizations (LRC). The use of acceleration factors for the LRM-method is subject to fewer restrictions than the LRC-method. In addition the former method does not require the square roots of the latter one. The natural factor formulation coupled with the LRM-method gives a far higher degree of precision than any of the other methods. Then, since each iteration of the QR-method requires an orthogonal factorization, which demands a larger volume of computation than the factorization adopted here, the present approach is competitive with the QR-method.

References

[1] H.L. Soriano, O método de Rutishauser modificado para o cálculo de autovalores em problemas estruturais, D.Sc. thesis, COPPE/Federal University of Rio de Janeiro (1979).

[2] J.H. Wilkinson, The Algebraic Eigenvalue Problem (Clarendon Press, Oxford, 1965).
[3] J.H. Wilkinson and C. Reinsch, Handbook for Automatic Computation, Vol. II (Springer-Verlag, Berlin, 1971).
[4] H.R. Schwarz, Numerical Analysis of Symmetric Matrices (Prentice-Hall, Englewood Cliffs, NJ, 1973).
[5] A. Jennings, Matrix Computation for Engineers and Scientists (Wiley, New York, 1977).
[6] D.K. Faddeev and V.N. Faddeeva, Computational Methods of Linear Algebra (Freeman, San Francisco, CA, 1963).
[7] L. Fox, An Introduction to Numerical Linear Algebra (Clarendon Press, Oxford, 1964).
[8] G.E. Forsythe and C.B. Moler, Computer Solution of Linear Algebraic Systems (Prentice-Hall, Englewood Cliffs, NJ, 1967).
[9] J.R. Roy, Numerical error in structural solutions, ASCE Structural Division, 1971.
[10] K.A. Braun and Th.L. Johnsen, Eigencomputation of symmetric hypermatrices using a generalization of the Householder method, Second International Conference on Structural Mechanics in Reactor Technology, Berlin, 1973.
[11] H.R. Schwarz, The eigenvalue problem $(\boldsymbol{A} - \lambda \cdot \boldsymbol{B})\boldsymbol{x} = \boldsymbol{0}$ for symmetric matrices of high order, Comput. Meths. Appl. Mech. Engrg. 3 (1974) 11–28.
[12] Th.L. Johnsen and J.R. Roy, On systems of linear equations of the form $\boldsymbol{A}^{\mathrm{t}} \cdot \boldsymbol{A} \cdot \boldsymbol{x} = \boldsymbol{b}$ error analysis and certain consequences for structural application, Comput. Meths. Appl. Mech. Engrg. 3 (1974) 357–374.
[13] G. Frik and Th.L. Johnsen, Note on the ill-conditioned eigenvalue problem in elastic vibrations, Comput. Meths. Appl. Mech. Engrg. 6 (1975) 65–77.
[14] O.E. Brönlund, Computation of the Cholesky factor of a stiffness matrix direct from the factor of its initial quadratic form, ISD Rept. No. 142, 1973.
[15] V. Wilhelmy, On the element stiffness factor formulation, Comput. Meths. Appl. Mech. Engrg. 11 (1977) 75–95.
[16] J.H. Argyris, Th.L. Johnsen and H.P. Mlejnek, On the natural factor in nonlinear analysis, ISD Rept. No. 242, Stuttgart, 1978.
[17] C.L.M. Prates, Obtenção do fator de Cholesky diretamente a partir da matriz de rigidez do elemento estrutural, M.Sc. thesis, COPPE/Federal University of Rio de Janeiro, Brazil, 1979.
[18] H.L. Soriano, Subestruturação com integração directa das equações de movimento da dinâmica estrutural, Report published by the National Laboratory of Civil Engineering, Lisbon, 1981.