THE LR ALGORITHM

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INTRODUCTION

The LR algorithm is a method for determining the eigenvalues of a matrix. The basic operation utilized by the algorithm is the triangularization of a matrix into the product of a unit lower-triangular matrix and an upper-triangular matrix. A unit lower-triangular matrix is a matrix whose diagonal elements are all 1, and whose elements above the diagonal are all zero. An upper-triangular matrix is one whose elements below the diagonal are all zero.

The algorithm will first be introduced in its simplest form. Following this a series of modifications will be developed to improve the accuracy of the algorithm and to accelerate its convergence. Gaussian elimination with pivoting is an elementary tool in developing these modifications. This process is a basic tool in numerical analysis problems dealing with systems of equations in matrix form. A development of Gaussian elimination may be found in any of the books listed in the bibliography.

THE LR ALGORITHM

The algorithm is based upon the triangular decomposition of a matrix A, given by

[1] $$A = LR$$

where L is a unit lower-triangular matrix and R is upper-triangular. If we now form the similarity transformation $L^{-1}AL$ on the matrix A, we have

[2] $$L^{-1}AL = L^{-1}(LR)L = RL \ .$$

Hence, if we decompose A and then multiply the factors in reverse order, we obtain a matrix similar to A. If we name the original matrix A_1, then the algorithm is defined by the equations

[3] $$A_{s-1} = L_{s-1}R_{s-1} \ , \qquad R_{s-1}L_{s-1} = A_s$$

Thus A_s is similar to A_{s-1} and by induction, to A_1. This process is repeated until we obtain a matrix A_s such that $L_s = I$, which means the diagonal elements of R_s are the eigenvalues of A_s. Since A_s is similar to A_1, these diagonal elements are also the eigenvalues of A_1. This then is the LR algorithm.

Since the algorithm is based upon the triangular decomposition of a matrix A, we shall introduce a method for the triangularization of a matrix. For the original matrix A, by [1],

$$A = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ & \cdots & & \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{bmatrix} =$$

$$\begin{bmatrix} 1 & 0 & \cdots & 0 \\ k_{21} & 1 & \cdots & 0 \\ & \cdots & & \\ k_{n1} & k_{n2} & \cdots & 1 \end{bmatrix} \begin{bmatrix} r_{11} & r_{12} & \cdots & r_{1n} \\ 0 & r_{22} & \cdots & r_{2n} \\ & \cdots & & \\ 0 & 0 & \cdots & r_{nn} \end{bmatrix}$$

Theorem 1. If the matrix A is triangularized such that $A = LR$, where L is unit lower-triangular and R is upper-triangular,

$$k_{ji} = \frac{\det(A_{ji})}{\det(A_{ii})}, \quad r_{ij} = \frac{\det(A_{ij})}{\det(A_{i-1,i-1})}, \; i = 1, \ldots, n$$

where A_{ii} is the leading principal minor of A of dimension $(i)x(i)$, and A_{ji} denotes this minor with its i^{th} row replaced by its j^{th} row.

If we partition the matrices shown above along the i^{th} row and i^{th} column, we have

$$\left[\begin{array}{c|c} A_{ii} & A_{i,n-i} \\ \hline A_{n-i,i} & A_{n-i,n-i} \end{array}\right] = \left[\begin{array}{c|c} L_{ii} & 0 \\ \hline K_{n-i,i} & L_{n-i,n-i} \end{array}\right] \left[\begin{array}{c|c} R_{ii} & R_{i,n-i} \\ \hline 0 & R_{n-i,n-i} \end{array}\right]$$

It follows that

$$[4] \qquad A_{ii} = L_{ii}R_{ii} \; .$$

Let A_{ji} denote the leading (i)x(i) principal submatrix of A with its i^{th} row replaced by its j^{th} row. Let the same definition hold for L_{ji}. It follows that

$$A_{ji} = L_{ji}R_{ii} \; .$$

Since L_{ii} is triangular, so is L_{ji}, but with k_{ji} on the diagonal. Thus

$$\det(L_{ji}) = k_{ji}$$

as all other diagonal elements are 1. Hence,

$$\det(A_{ji}) = k_{ji} \det(R_{ii}) \; .$$

When i = j,

$$\det(A_{ii}) = \det(R_{ii}) \; .$$

Hence,

$$k_{ji} = \frac{\det(A_{ji})}{\det(A_{ii})} \; , \; i = 1, 2, \ldots, n.$$

Similarly, we can find an expression for the r_{ij}, using transposes.

$$A'_{ii} = R'_{ii}L'_{ii} \; , \qquad A'_{ji} = R'_{ji}L'_{ii}$$

where A' is the transpose of A. Note that

$$\det(L'_{ii}) = 1 .$$

Therefore

$$\det(A'_{ii}) = \det(R'_{ii}) , \quad \det(A'_{ji}) = \det(R'_{ji}) .$$

By the definition of R'_{ji},

$$\det(R'_{ji}) = \frac{r_{ij} \det(R'_{ii})}{r_{ii}}$$

and

$$r_{ii} = \frac{\det(R_{ii})}{\det(R_{i-1,i-1})} .$$

Therefore,

$$r_{ij} = \frac{r_{ii} \det(R'_{ji})}{\det(R'_{ii})} = \frac{\det(R_{ii})\det(R'_{ji})}{\det(R_{i-1,i-1})\det(R'_{ii})}$$

so that

$$r_{ij} = \frac{\det(A_{ii})\det(A'_{ji})}{\det(A_{i-1,i-1})\det(A'_{ii})} = \frac{\det(A'_{ji})}{\det(A_{i-1,i-1})} .$$

Since $A'_{ji} = A_{ij}$,

$$r_{ij} = \frac{\det(A_{ij})}{\det(A_{i-1,i-1})} ,$$

where $\det(A_{00}) = 1$. Thus

$$r_{ij} = \frac{\det(A_{ij})}{\det(A_{i-1,i-1})} , \quad k_{ji} = \frac{\det(A_{ji})}{\det(A_{ii})} .$$

For a simple 3x3 matrix A,

$$A = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix}$$

$$L = \begin{bmatrix} 1 & 0 & 0 \\ \dfrac{\det(A_{21})}{\det(A_{11})} & 1 & 0 \\ \dfrac{\det(A_{31})}{\det(A_{11})} & \dfrac{\det(A_{32})}{\det(A_{22})} & 1 \end{bmatrix}$$

$$R = \begin{bmatrix} \det(A_{11}) & \det(A_{12}) & \det(A_{13}) \\ 0 & \dfrac{\det(A_{22})}{\det(A_{11})} & \dfrac{\det(A_{23})}{\det(A_{11})} \\ 0 & 0 & \dfrac{\det(A_{33})}{\det(A_{22})} \end{bmatrix}$$

With this notation established, we return to the algorithm. The following assumptions concerning the matrix A will now be made. We assume the eigenvalues are real and of different absolute value and that the leading principal minors of X and Y are non-zero, where X is the matrix of right-hand eigenvectors of A and $Y = X^{-1}$.

Theorem 2. If $A = LR$, under the restrictions just stated, $L_s \to I$ and

[5] $$R_s \to A_s \to \begin{bmatrix} \lambda_1 & & & & \\ & \lambda_2 & & X & \\ & & \cdot & & \\ & 0 & & \cdot & \\ & & & & \lambda_n \end{bmatrix} \text{ as } S \to \infty$$

where X denotes the possible non-zero elements of an upper-triangular matrix.

To prove this result, we establish relations between successive iterations which will be used extensively. By [3],

$$A_s = L_{s-1}^{-1} A_{s-1} L_{s-1} .$$

Repeated application of this result yields

[6] $$A_s = L_{s-1}^{-1} L_{s-2}^{-1} \cdots L_2^{-1} L_1^{-1} A_1 L_1 L_2 \cdots L_{s-2} L_{s-1}$$

or

[7] $$L_1 L_2 \cdots L_{s-1} A_s = A_1 L_1 L_2 \cdots L_{s-1} .$$

Now define matrices T_s and U_s by

[8] $$T_s = L_1 L_2 \cdots L_s \text{ and } U_s = R_s R_{s-1} \cdots R_1 .$$

These matrices are unit lower-triangular and upper-triangular respectively. Consider the product T_sU_s.

$$
\begin{aligned}
T_sU_s &= L_1L_2 \cdots L_{s-1}(L_sR_s)R_{s-1} \cdots R_2R_1 \\
&= L_1L_2 \cdots L_{s-1}A_sR_{s-1} \cdots R_2R_1 \\
&= A_1L_1L_2 \cdots (L_{s-1}R_{s-1}) \cdots R_2R_1 \\
&= A_1L_1L_2 \cdots L_{s-2}(A_{s-1})R_{s-2} \cdots R_2R_1 \\
&= A_1^2L_1L_2 \cdots (L_{s-2}R_{s-2}) \cdots R_2R_1 \\
&= A_1^2L_1L_2 \cdots L_{s-3}(A_{s-2})R_{s-3} \cdots R_2R_1 \\
&= A_1^3L_1L_2 \cdots (L_{s-3}R_{s-3}) \cdots R_2R_1 \\
&\quad \cdots\cdots\cdots\cdots \\
&= A_1^s
\end{aligned}
$$

Hence, repeated application of [7] yields

[9] $$T_sU_s = A_1^s$$

so that T_sU_s gives the triangular decomposition of A_1^s.

PROOF OF THE CONVERGENCE OF A_s

Equation [7] is a fundamental tool in the analysis. We shall prove that if the eigenvalues λ_i of A_1 satisfy the relation

$$|\lambda_1| > |\lambda_2| > |\lambda_3| > \ldots. > |\lambda_n|$$

then in general the results of [5] are true.

Before giving a formal proof, we consider an example of a matrix of order three. Note, that if $X^{-1}AX = \mathrm{diag}(\lambda_i)$, where the λ_i are the eigenvalues of A, then X is a matrix of righthand eigenvectors of A, written as column vectors. This comes from the relation $AX = \lambda_i X$, where X denotes the eigenvector corresponding to λ_i. For simplicity, we denote the matrix X of righthand eigenvectors in the form

$$X = \begin{bmatrix} x_{11} & x_{12} & x_{13} \\ x_{21} & x_{22} & x_{23} \\ x_{31} & x_{32} & x_{33} \end{bmatrix}$$

and its inverse Y by

$$X^{-1} = Y = \begin{bmatrix} y_{11} & y_{12} & y_{13} \\ y_{21} & y_{22} & y_{23} \\ y_{31} & y_{32} & y_{33} \end{bmatrix}$$

If we denote $T_s U_s = A_1^s = B$, then

$$B = A_1^s = X \begin{bmatrix} \lambda_1^s & & \\ & \lambda_2^s & \\ & & \lambda_3^s \end{bmatrix} X^{-1} = \begin{bmatrix} c_{11} & c_{12} & c_{13} \\ c_{21} & c_{22} & c_{23} \\ c_{31} & c_{32} & c_{33} \end{bmatrix}$$

where

$$c_{11} = \lambda_1^s x_{11} y_{11} + \lambda_2^s x_{12} y_{21} + \lambda_3^s x_{13} y_{31}$$

$$c_{21} = \lambda_1^s x_{21} y_{11} + \lambda_2^s x_{22} y_{21} + \lambda_3^s x_{23} y_{31}$$

$$c_{31} = \lambda_1^s x_{31} y_{11} + \lambda_2^s x_{32} y_{21} + \lambda_3^s x_{33} y_{31}$$

$$c_{12} = \lambda_1^s x_{11} y_{12} + \lambda_2^s x_{12} y_{22} + \lambda_3^s x_{13} y_{32}$$

$$c_{22} = \lambda_1^s x_{21} y_{12} + \lambda_2^s x_{22} y_{22} + \lambda_3^s x_{23} y_{32}$$

$$c_{32} = \lambda_1^s x_{31} y_{12} + \lambda_2^s x_{32} y_{22} + \lambda_3^s x_{33} y_{32}$$

$$c_{13} = \lambda_1^s x_{11} y_{13} + \lambda_2^s x_{12} y_{23} + \lambda_3^s x_{13} y_{33}$$

$$c_{23} = \lambda_1^s x_{21} y_{13} + \lambda_2^s x_{22} y_{23} + \lambda_3^s x_{23} y_{33}$$

$$c_{33} = \lambda_1^s x_{31} y_{13} + \lambda_2^s x_{32} y_{23} + \lambda_3^s x_{33} y_{33}$$

Now $T_s U_s$ is the triangular decomposition of A_1^s and hence the elements of the first column of T_s will correspond to the elements of the first column of L given on page 6. They are

$$t_{11}^{(s)} = 1 = \frac{\det(B_{11})}{\det(B_{11})} \quad .$$

$$t_{21}^{(s)} = \frac{\lambda_1^s x_{21} y_{11} + \lambda_2^s x_{22} y_{21} + \lambda_3^s x_{23} y_{31}}{\lambda_1^s x_{11} y_{11} + \lambda_2^s x_{12} y_{21} + \lambda_3^s x_{13} y_{31}} = \frac{\det(B_{21})}{\det(B_{11})}$$

$$t_{31}^{(s)} = \frac{\lambda_1^s x_{31} y_{11} + \lambda_2^s x_{32} y_{21} + \lambda_3^s x_{33} y_{31}}{\lambda_1^s x_{11} y_{11} + \lambda_2^s x_{12} y_{21} + \lambda_3^s x_{13} y_{31}} = \frac{\det(B_{31})}{\det(B_{11})}$$

Due to the ordering of the magnitude of the eigenvalues, λ_1^s will dominate the denominator as $s \to \infty$. Hence if $x_{11} y_{11} \neq 0$,

$$t_{21}^{(s)} = x_{21}/x_{11} + O(\lambda_2/\lambda_1)^s$$

$$t_{31}^{(s)} = x_{31}/x_{11} + O(\lambda_2/\lambda_1)^s$$

where $O(\lambda_2/\lambda_1)^s$ is a term(s) of order $(\lambda_2/\lambda_1)^s$, which approaches zero since $|\lambda_1| > |\lambda_2|$.

Thus the elements of the first column of T_s approach the corresponding elements in the triangular decomposition of X. Similarly, for the elements of the second column of T_s, we have

$$t_{22}^{(s)} = 1 = \frac{\det(B_{22})}{\det(B_{22})}$$

[10] $$t_{32}^{(s)} = \frac{\det(B_{32})}{\det(B_{22})} = \frac{(\lambda_1\lambda_2)^s a_1 + (\lambda_1\lambda_3)^s a_2 + (\lambda_2\lambda_3)^s a_3}{(\lambda_1\lambda_2)^s b_1 + (\lambda_1\lambda_3)^s b_2 + (\lambda_2\lambda_3)^s b_3}$$

where

$$a_1 = (x_{11}x_{32} - x_{31}x_{12})(y_{11}y_{22} - y_{21}y_{12})$$

$$a_2 = (x_{11}x_{33} - x_{31}x_{13})(y_{11}y_{32} - y_{31}y_{12})$$

$$a_3 = (x_{12}x_{33} - x_{32}x_{13})(y_{21}y_{32} - y_{31}y_{22})$$

$$b_1 = (x_{11}x_{22} - x_{21}x_{12})(y_{11}y_{22} - y_{21}y_{12})$$

$$b_2 = (x_{11}x_{23} - x_{21}x_{13})(y_{11}y_{32} - y_{31}y_{12})$$

$$b_3 = (x_{12}x_{23} - x_{13}x_{22})(y_{21}y_{32} - y_{31}y_{22}) \quad .$$

If we now divide numerator and denominator by $(\lambda_1\lambda_2)^s$

$$t_{32}^{(s)} = \frac{a_1 + (\lambda_3/\lambda_2)^s a_2 + (\lambda_3/\lambda_1)^s a_3}{b_1 + (\lambda_3/\lambda_2)^s b_2 + (\lambda_3/\lambda_1)^s b_3} \quad .$$

Hence

$$t_{32}^{(s)} = \frac{x_{11}x_{32} - x_{31}x_{12}}{x_{11}x_{22} - x_{21}x_{12}} + O(\lambda_3/\lambda_2)^s$$

provided $(x_{11}x_{22} - x_{21}x_{12})(y_{11}y_{22} - y_{21}y_{12}) \neq 0$. We can see from [10] that the limiting value of $t_{32}^{(s)}$ is equal to the corresponding element obtained in the triangular decomposition of X. We have thus established that if

$$X = TU$$

then, provided $x_{11}y_{11} \neq 0$ and $(x_{11}x_{22} - x_{21}x_{12})(y_{11}y_{22} - y_{21}y_{12}) \neq 0$,

$$T_s \to T \ .$$

Thus, we have shown in this simple example that the matrix T_s tends to the unit lower-triangular matrix obtained from the triangular decomposition of the matrix X of eigenvectors, provided the leading minors of X and Y are non-zero. Now we shall prove Theorem 2 in general for a matrix with distinct eigenvalues. If we write

$$T_s U_s = A_1^s = B$$

then we have

$$t_{ji}^{(s)} = \det(B_{ji})/\det(B_{ii})$$

as we have proved earlier for s = 1.

From the relation

$$B = A_1^s = X \operatorname{diag}(\lambda_i^s)\, X^{-1}$$

we have that

$$B_{ji} = \begin{bmatrix} x_{11} & x_{12} & \cdots & x_{1n} \\ x_{21} & x_{22} & \cdots & x_{2n} \\ & \cdots\cdots & & \\ x_{i-1,1} & x_{i-1,2} & \cdots & x_{i-1,n} \\ x_{j1} & x_{j2} & \cdots & x_{jn} \end{bmatrix} \begin{bmatrix} \lambda_1^s y_{11} & \lambda_1^s y_{12} & \cdots & \lambda_1^s y_{1i} \\ \lambda_2^s y_{21} & \lambda_2^s y_{22} & \cdots & \lambda_2^s y_{2i} \\ & \cdots\cdots & & \\ & \cdots\cdots & & \\ \lambda_n^s y_{n1} & \lambda_n^s y_{n2} & \cdots & \lambda_n^s y_{ni} \end{bmatrix} \tag{11}$$

By the theorem of corresponding matrices (chapter 1, section 15)[1], $\det(B_{ji})$ is equal to the sum of the products of the corresponding

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1. See Bibliography

i-rowed minors of the two matrices on the right in [11]. Hence we may write

$$t_{ji}^{(s)} = \frac{\sum x^{(j)}_{p_1p_2\cdots p_i} y^{(i)}_{p_1p_2\cdots p_i} (\lambda_{p_1}\lambda_{p_2}\cdots\lambda_{p_i})^s}{\sum x^{(i)}_{p_1p_2\cdots p_i} y^{(i)}_{p_1p_2\cdots p_i} (\lambda_{p_1}\lambda_{p_2}\cdots\lambda_{p_i})^s}$$

where $x^{(j)}_{p_1p_2\cdots p_i}$ is the i-rowed minor consisting of rows 1, 2, ..., i-1 and j and columns p_1, p_2, ..., p_i of X and $y^{(i)}_{p_1p_2\cdots p_i}$ is the i-rowed minor consisting of rows p_1, p_2, ..., p_i and columns 1, 2, ..., i of Y.

The dominant terms in the numerator and denominator are those associated with $(\lambda_1\lambda_2 \ldots\lambda_i)^s$ providing the corresponding coefficients are non-zero. Thus, the dominant term in the denominator is

$$\det(X_{ii}) \det(Y_{ii})(\lambda_1\lambda_2 \ldots \lambda_i)^s$$

where X_{ii} and Y_{ii} are the leading principal submatrices of order i. If $\det(X_{ii}) \det(Y_{ii})$ is non-zero, we have

$$t_{ji}^{(s)} \to \frac{\det(X_{ji}) \det(Y_{ii})}{\det(X_{ii}) \det(Y_{ii})} = \frac{\det(X_{ji})}{\det(X_{ii})}$$

showing that $T_s \to T$, where $T = XU^{-1}$. We have from [8], [6], and [7] that

$$A_s = T_{s-1}^{-1}A_1T_{s-1} \to T^{-1}A_1T = UX^{-1}AXU^{-1}$$

$$= U \operatorname{diag}(\lambda_i)\, U^{-1}$$

showing that the limiting A_s is upper-triangular with diagonal elements λ_i.

From the relation $L_s = T_{s-1}^{-1} T_s$ and equation [12] it can be proved in a similar and quite tedious argument that

$$k_{ij}^{(s)} = O(\lambda_i/\lambda_j)^s \quad \text{as} \quad s \to \infty \ .$$

From this we deduce, using the relation $A_s = L_s R_s$, that

$$a_{ij} = O(\lambda_i/\lambda_j)^s \quad \text{as} \quad s \to \infty \ .$$

Hence, if the separation of some of the eigenvalues is poor, the convergence may be quite slow.

It should be noted that in establishing these results, the following assumptions have been made, either explicitly or implicitly.

i). The eigenvalues are real and of different magnitude.

ii). The triangular decomposition exists at every stage. It is relatively simple to construct matrices, not otherwise exceptional, for which this is not true. For example,

$$A = \begin{bmatrix} 0 & 1 \\ -3 & 4 \end{bmatrix} .$$

This matrix has eigenvalues 1 and 3 but has no triangular decomposition. However, this case can be handled through the use of interchanges, which we will introduce later.

iii). The leading principal minors of X and Y are all non-zero.

POSITIVE DEFINITE HERMITIAN MATRICES

When A_1 is a positive definite Hermitian matrix we can remove the restrictions of the last section. Thus

$$A_1 = X \operatorname{diag}(\lambda_i) X^H , \text{ where } X^H = X^{-1}$$

and where X is unitary and the λ_i are real and positive. Hence, equation [10] becomes

$$t_{ji}^{(s)} = \frac{\sum X^{(j)}_{p_1p_2\cdots p_i} \overline{X}^{(i)}_{p_1p_2\cdots p_i} (\lambda_{p_1}\lambda_{p_2}\cdots\lambda_{p_i})^s}{\sum |X_{p_1p_2\cdots p_i}|^2 (\lambda_{p_1}\lambda_{p_2}\cdots\lambda_{p_i})^s} .$$

Now consider the class of aggregates $p_1p_2\cdots p_i$ for which $X^{(i)}_{p_1p_2\cdots p_i} \neq 0$. Let $q_1q_2\cdots q_i$ be a member of this class such that $\lambda_{q_1}\lambda_{q_2}\cdots\lambda_{q_i}$ has a value greater than that of any other member. Thus the denominator is clearly dominated by the term(s) in $(\lambda_{q_1}\lambda_{q_2}\cdots\lambda_{q_i})^s$.

As for the numerator, we know from our definition of $q_1q_2\cdots q_i$ that no term exceeds the magnitude of $(\lambda_{q_1}\lambda_{q_2}\cdots\lambda_{q_i})^s$, but this term may have a zero coefficient. Hence, $t_{ji}^{(s)}$ tends to a limit which may be zero.

No assumptions are made about the principal minors of X and hence we cannot assert that the limiting T_s is the matrix obtained in the triangular decomposition of X. Accordingly, we proceed by writing

$$T_s \to T_\infty$$

so that

$$L_s = T_{s-1}^{-1} T_s \to T_\infty^{-1} T_\infty = I \ .$$

Further,

$$A_s = T_{s-1}^{-1} A_1 T_{s-1} \to T_\infty^{-1} A_1 T_\infty \qquad [13]$$

so that A_s tends to a limit, say A_∞. Now

$$R_s = L_s^{-1} A_s \to I T_\infty^{-1} A_1 T_\infty ,$$

and hence R_s tends to the same limit as A_s. Since R_s is triangular for all s, this limit must be triangular also. It must have the eigenvalues of A_1 in some order on its diagonal, since it is similar, from [13], to A_1.

Note that the proof is unaffected by the presence of multiple eigenvalues or by the vanishing of some of the leading principal minors of X, though the λ_i may not appear in decreasing order on the diagonal of A^s.

It is now advisable to assess the value of the LR algorithm as a practical technique. It does not appear to be very adequate for the following reasons:

i). Matrices exist which have no triangular decomposition, in spite of the fact that their eigenproblem is well-conditioned. Without some sort of modification, such matrices cannot be handled by the LR algorithm. Further, there is a much larger class of matrices whose triangular decomposition is numerically unstable. This instability can arise at any step of the algorithm, which may lead to considerable inaccuracy in the computation of the eigenvalues. A method to eliminate this instability will be discussed in the section covering interchanges.

ii). The volume of computation is very high. The method involves $(n-1)n^2$ multiplications at each step of the process. A method of reducing the amount of computation will be discussed in the section on Hessenberg matrices.

iii). The convergence of the subdiagonal elements of L_s depends upon the ratio $(\lambda_{r+1}/\lambda_r)$ and will be very slow if separation of the eigenvalues is poor. This problem is discussed in the section covering acceleration of convergence.

Thus if the LR algorithm is to be useful, it must be modified to meet these criticisms. To accomplish this, we will use elementary matrices which interchange or combine multiples of the rows and columns of A.

INTRODUCTION OF INTERCHANGES

In triangular decomposition numerical stability is maintained by the introduction of interchanges if necessary. Consider an analogous modification of the LR algorithm.

If A is any matrix, by Gaussian elimination, there exists a product of elementary matrices, P, such that

$$PA = R \tag{14}$$

where R is upper-triangular. We can therefore complete a similarity transformation on A by post-multiplying R by P^{-1} and have

$$PAP^{-1} = RP^{-1} \ . \tag{15}$$

In particular, when there are no interchanges necessary the matrix P equals the matrix L^{-1} and [14] becomes

$$L^{-1}A = R \ .$$

In this case the matrix on the right of [15] is RL.

As a numerical example of the modified process, we take a 3x3 matrix to illustrate non-convergence of the orthodox LR algorithm. The matrix A_1, the corresponding λ_i, and the X and Y matrices are:

$$A_1 = \begin{bmatrix} 1 & -1 & 1 \\ 4 & 6 & -1 \\ 4 & 4 & 1 \end{bmatrix} \qquad \begin{aligned} \lambda_1 &= 5 \\ \lambda_2 &= 2 \\ \lambda_3 &= 1 \end{aligned}$$

$$X = \begin{bmatrix} 0 & -1 & -1 \\ 1 & 1 & 1 \\ 1 & 0 & 1 \end{bmatrix} \qquad Y = \begin{bmatrix} 1 & 1 & 0 \\ 0 & 1 & -1 \\ -1 & -1 & 1 \end{bmatrix}$$

The leading principal minor of X is zero. Hence we cannot be sure that the orthodox process converges, or, if it does, whether it will yield the eigenvalues in descending order. In fact, in this case the elements of T_s diverge. In Table 1, we have shown the results of the first three steps of the LR process, and from the form of A_s divergence is obvious.

TABLE 1

$$A_2 = \begin{bmatrix} 1 & -0.2 & 1 \\ 20 & 6 & -5 \\ 4 & 0.8 & 1 \end{bmatrix} \qquad A_3 = \begin{bmatrix} 1 & -0.04 & 1 \\ 100 & 6 & -25 \\ 4 & 0.16 & 1 \end{bmatrix} \qquad A_4 = \begin{bmatrix} 1 & -0.008 & 1 \\ 500 & 6 & -125 \\ 4 & 0.032 & 1 \end{bmatrix}$$

Below: LR with interchanges

$$A_2 = \begin{bmatrix} 6 & 3.2 & -1 \\ -1.25 & 1 & 1.25 \\ 1 & 0.8 & 1 \end{bmatrix} \qquad A_3 = \begin{bmatrix} 5.167 & 3.040 & -1.00 \\ -0.174 & 1.833 & 1.042 \\ 0.167 & 0.160 & 1.000 \end{bmatrix} \qquad A_4 = \begin{bmatrix} 5.032 & 3.008 & -1.00 \\ -0.03 & 1.968 & 1.008 \\ 0.032 & 0.032 & 1.000 \end{bmatrix}$$

$$A_\infty$$

$$\begin{bmatrix} 5 & 3 & -1 \\ 0 & 2 & 1 \\ 0 & 0 & 1 \end{bmatrix}$$

Table 1 also gives the results obtained using the modified process. The first step in detail yields:

$$\begin{bmatrix} 1 & -1 & 1 \\ 4 & 6 & -1 \\ 4 & 4 & 1 \end{bmatrix} \overset{\longleftrightarrow}{R(1,2)} \begin{bmatrix} 4 & 6 & -1 \\ 1 & -1 & 1 \\ 4 & 4 & 1 \end{bmatrix} \overset{\longleftrightarrow}{R2-(1/4)R1} \begin{bmatrix} 4 & 6 & -1 \\ 0 & -2.5 & 1.25 \\ 4 & 4 & 1 \end{bmatrix}$$

where R(1,2) indicates an interchange of rows 1 and 2, and R2-(1/4)R1 indicates the subtraction of 1/4 the elements of row 1 from the corresponding elements in row 2.

$$\begin{bmatrix} 4 & 6 & -1 \\ 0 & -2.5 & 1.25 \\ 4 & 4 & 1 \end{bmatrix} \overset{\longleftrightarrow}{R3-R1} \begin{bmatrix} 4 & 6 & -1 \\ 0 & -2.5 & 1.25 \\ 0 & -2 & 2 \end{bmatrix}$$

$$\overset{\longleftrightarrow}{R3-.8R2} \begin{bmatrix} 4 & 6 & -1 \\ 0 & -2.5 & 1.25 \\ 0 & 0 & 1 \end{bmatrix} = R$$

$$\begin{bmatrix} 4 & 6 & -1 \\ 0 & -2.5 & 1.25 \\ 0 & 0 & 1 \end{bmatrix} \xleftrightarrow[C(1,2)]{} \begin{bmatrix} 6 & 4 & -1 \\ -2.5 & 0 & 1.25 \\ 0 & 0 & 1 \end{bmatrix}$$

$$\xleftrightarrow[C1+(1/4)C2]{} \begin{bmatrix} 7 & 4 & -1 \\ -2.5 & 0 & 1.25 \\ 0 & 0 & 1 \end{bmatrix} \xleftrightarrow[C1+C3]{} \begin{bmatrix} 6 & 4 & -1 \\ -1.25 & 0 & 1.25 \\ 1 & 0 & 1 \end{bmatrix}$$

$$\xleftrightarrow[C2+.8C3]{} \begin{bmatrix} 6 & 3.2 & -1 \\ -1.25 & 1 & 1.25 \\ 1 & .8 & 1 \end{bmatrix} = A_2$$

The choice of which elements to interchange in the first step is an important one. Since we have two equal elements in the first column, the second row is interchanged with the first. This choice is made so that the largest diagonal element, 6, will become the leading element of the matrix after the corresponding column interchange. This is done because we want the eigenvalues in descending order on the diagonal.

Only one interchange is necessary in the first step. In the subsequent steps we are using the orthodox LR technique, as no more interchanges are necessary. The matrix A_s converges very rapidly to an upper-triangular matrix. The use of interchanges has not only yielded convergence, but also gave the eigenvalues in descending order.

The use of interchanges has given us numerical stability in triangular decomposition for a simple reason. As may be noted in the simple example on page 6, triangularization utilizes a division by $\det(A_{11})$. The introduction of interchanges has made $\det(A_{11})$ greater than or equal to all other elements in the first column, hence, the first and second columns of L will become increasingly smaller. Without this modification, the orthodox LR technique performs this division without regard to the relative size of a_{11}, and hence, as is seen in Table 1, elements may increase in size.

THE UPPER HESSENBERG FORM

It would seem that the volume of work involved is still prohibitive when A is a matrix with few zero elements. If, however, A is of a condensed form which is invariant with respect to the LR algorithm, then the volume of work might well be reduced.

The major form which meets this requirement is the upper Hessenberg form, which is invariant with respect to the modified LR algorithm, and therefore a fortiori with respect to the orthodox process. We first reduce a matrix to upper Hessenberg form. We define a matrix to be upper Hessenberg form if $a_{ij} = 0$ for $i \geq j+2$. This reduction may be accomplished in the following manner. We will utilize a matrix, call it N, with the following characteristics: N is unit lower-triangular, and the elements of the first column, except for the diagonal element, are zero. Hence, N has the form, for n = 5,

$$N = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & n_{32} & 1 & 0 & 0 \\ 0 & n_{42} & n_{43} & 1 & 0 \\ 0 & n_{52} & n_{53} & n_{54} & 1 \end{bmatrix} .$$

For our initial matrix A, we now form the equation

$$AN = NH \tag{16}$$

where H is upper Hessenberg.

$$\overset{[A]}{\begin{bmatrix} x & x & x & x & x \\ x & x & x & x & x \\ x & x & x & x & x \\ x & x & x & x & x \\ x & x & x & x & x \end{bmatrix}} \overset{[N]}{\begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & n_{32} & 1 & 0 & 0 \\ 0 & n_{42} & n_{43} & 1 & 0 \\ 0 & n_{52} & n_{53} & n_{54} & 1 \end{bmatrix}}$$

$$= \overset{[N]}{\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & n_{32} & 1 & 0 \\ 0 & n_{42} & n_{43} & 1 \\ 0 & n_{52} & n_{53} & n_{54} \end{bmatrix}} \overset{[H]}{\begin{bmatrix} 0 & h & h & h & h & h \\ 0 & h & h & h & h & h \\ 0 & 0 & h & h & h & h \\ 0 & 0 & 0 & h & h & h \\ 1 & 0 & 0 & 0 & h & h \end{bmatrix}}$$

where x and h denote possible non-zero elements. The elements of N and H can be computed column by column. Multiplication of [16] by N^{-1} yields

$$N^{-1}AN = H \ .$$

Hence, A is similar to H, an upper Hessenberg matrix. For a further discussion of this method, see Wilkinson (chapter 6, section 11)[2].

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2. See Bibliography

We now return to the invariance of the upper Hessenberg form with respect to the LR algorithm. We want to show that after one complete step of the algorithm A_2 is of upper Hessenberg form. This is done by induction. This can be done in this manner since the elementary operations used to triangularize A_1 will involve only rows 1 and 2 at step 1, only rows 2 and 3 at step 2, and so forth. Hence, after (r-1) steps of the post-multiplication by these factors, only the first (r-1) columns of the matrix will have been affected. Thus, assume that after (r-1) steps the matrix is of upper Hessenberg form in its first (r-1) columns and triangular in the remaining columns. For the case n = 6, r = 4, it is of the form

$$\begin{bmatrix} x & x & x & x & x & x \\ x & x & x & x & x & x \\ & x & x & x & x & x \\ & & x & x & x & x \\ & & & & x & x \\ & & & & & x \end{bmatrix}$$

where x denotes possible non-zero elements, and the elements not shown are all zero. The next step will be the interchange of columns r and (r+1) if rows r and (r+1) were interchanged; if not, there is no effect. The resulting matrix is therefore of the form (a) or (b) shown below.

$$
(a)\ \begin{bmatrix} x & x & x & x & x & x \\ x & x & x & x & x & x \\ & x & x & x & x & x \\ & & x & x & x & x \\ & & & x & 0 & x \\ & & & & & x \end{bmatrix}, \quad (b)\ \begin{bmatrix} x & x & x & x & x & x \\ x & x & x & x & x & x \\ & x & x & x & x & x \\ & & x & x & x & x \\ & & & & x & x \\ & & & & & x \end{bmatrix}
$$

where (a) shows the effect of an interchange.

Next a multiple of column $(r+1)$ will be added to column r and the resulting matrix will be of form (c), from (a), or (d), from (b).

$$
(c)\ \begin{bmatrix} x & x & x & x & x & x \\ x & x & x & x & x & x \\ & x & x & x & x & x \\ & & x & x & x & x \\ & & & x & 0 & x \\ & & & & & x \end{bmatrix}, \quad (d)\ \begin{bmatrix} x & x & x & x & x & x \\ x & x & x & x & x & x \\ & x & x & x & x & x \\ & & x & x & x & x \\ & & & x & x & x \\ & & & & & x \end{bmatrix}
$$

In either case the matrix is of upper Hessenberg form in its first r columns and triangular otherwise; the extra zero element in (c) being of no significance. Hence, the upper-Hessenberg form is invariant with respect to the modified algorithm.

There are $n^2/2$ multiplications in the reduction to triangular form and $n^2/2$ in the post-multiplication, yielding n^2 steps in one complete cycle of the LR algorithm, compared with $(n-1)n^2$ for a full matrix.

ACCELERATION OF CONVERGENCE

Although a preliminary reduction to upper Hessenberg form reduces the volume of computation considerably, the modified LR method will still be somewhat uneconomical without improving the rate of convergence.

As we have seen for a general matrix, the elements in positions (i,j), $i > j$, tend to zero as $(\lambda_i/\lambda_j)^s$ does. For Hessenberg matrices the only non-zero subdiagonal elements are those in positions (i+1,i). Now consider the matrix $(A - pI)$, where p is some real number. We will discuss a method of selecting p later.

The matrix $(A - pI)$ has eigenvalues $(\lambda_i - p)$ and, for example, the element $a_{n,n-1}^{(s)}$ tends to zero as $[(\lambda_n - p)/(\lambda_{n-1} - p]^s$ does. If p is a good approximation to λ_n, the element $a_{n,n-1}^{(s)}$ will decrease rapidly. Thus it would be to our advantage to use $(A_s - pI)$ rather than A_s.

Note, in particular, if p is exactly equal to λ_n, then the element $a_{n,n-1}^{(s)}$ would be zero after one iteration. This may be seen by considering the triangularization process. None of the pivots (the diagonal elements of the matrix R) can be zero except the last, because at each stage in the reduction the pivot is either $a_{i+1,i}$ or some other non-zero number and we are assuming that no $a_{i+1,i}$ is zero originally. Hence, since the determinant of $(A - \lambda_n I)$ is zero, and R is the form

$$\begin{bmatrix} x & x & x & x & x \\ & x & x & x & x \\ & & x & x & x \\ & & & x & x \\ & & & & 0 \end{bmatrix},$$

the whole of the last row being null. The subsequent post-multiplication merely combines columns and after the iteration the matrix is of the form

$$\begin{bmatrix} x & x & x & x & x \\ x & x & x & x & x \\ & x & x & x & x \\ & & x & x & x \\ & & & 0 & 0 \end{bmatrix}.$$

The previous discussion suggests the following modification of the LR method. At the s^{th} stage we perform a triangulr decomposition of $(A_s - k_sI)$, where k_s is some suitable value, rather than of A_s. We therefore produce the sequence of matrices defined by

$$A_s - k_sI = L_sR_s$$

$$R_sL_s + k_sI = A_{s+1} .$$

Thus,

$$A_{s+1} = R_sL_s + k_sI = L_s^{-1}(A_s - k_sI)L_s + k_sI = L_s^{-1}A_sL_s$$

and hence the matrices A_s are again similar to A_1. In fact

$$A_{s+1} = L_s^{-1}A_sL_s = L_s^{-1}L_{s-1}^{-1}A_{s-1}L_{s-1}L_s = L_s^{-1} \dots L_s^{-1}L_1^{-1}A_1L_1L_2 \dots L_s$$

or

$$L_1L_2 \dots L_sA_{s+1} = A_1L_1L_2 \dots L_s .$$

This formulation of the modification is usually described as LR with shifts of origin and restoring, because the shift is added back at each stage. We have

$$\begin{aligned}
L_1L_2 \dots L_{s-1}&(L_sR_s)R_{s-1} \dots R_2R_1 \\
&= L_1L_2 \dots L_{s-1}(A_s - k_sI)R_{s-1} \dots R_2R_1 \\
&= (A_1 - k_sI)L_1L_2 \dots (L_{s-1}R_{s-1}) \dots R_2R_1 \\
&= (A_1 - k_sI)(A_1 - k_{s-1}I)L_1L_2 \dots L_{s-2}R_{s-2} \dots R_2R_1 \\
&= (A_1 - k_sI)(A_1 - k_{s-1}I) \dots (A_1 - k_1I) .
\end{aligned}$$

Hence, writing

$$T_s = L_1L_2 \dots L_s, \qquad U_s = R_s \dots R_2R_1$$

we see that T_sU_s gives the triangular decomposition of

$$\prod_{i=1}^{s} (A_1 - k_iI) ,$$

the order of the factors being immaterial.

In a practical sense we are now faced with selecting a suitable sequence of k_s so as to give rapid convergence. We expect, in the matrix A_s, that $a_{n,n-1}^{(s)}$ and $a_{nn}^{(s)}$ will approach zero and λ_n respectively. Hence it is reasonable to take $k_s = a_{nn}^{(s)}$ as soon as $a_{n,n-1}^{(s)}$ becomes < 1 or $a_{nn}^{(s)}$ indicates it is converging. In fact, it is simple to show that when $a_{n,n-1}^{(s)}$ is of order ε then, if we choose $k_s = a_{nn}^{(s)}$, we have

$$a_{n,n-1}^{(s+1)} = O(\varepsilon^2) \ .$$

For $(A_s - a_{nn}^{(s)}I)$ with $n = 6$, is of the form shown in matrix (a) below.

(a)

$$\begin{bmatrix} x & x & x & x & x & x \\ x & x & x & x & x & x \\ & x & x & x & x & x \\ & & x & x & x & x \\ & & & x & x & x \\ & & & & \varepsilon & 0 \end{bmatrix}$$

(b)

$$\begin{bmatrix} x & x & x & x & x & x \\ & x & x & x & x & x \\ & & x & x & x & x \\ & & & x & x & x \\ & & & & a & b \\ & & & & \varepsilon & 0 \end{bmatrix}$$

(c)

$$\begin{bmatrix} x & x & x & x & x & x \\ & x & x & x & x & x \\ & & x & x & x & x \\ & & & x & x & x \\ & & & & a & b \\ & & & & & -b\varepsilon/a \end{bmatrix}$$

Consider now the reduction of $(A_s - a_{nn}^{(s)}I)$ to triangular form by the use of Gaussian elimination with interchanges. Matrix (b) above indicates the form of the matrix when only the last row remains to be reduced. The element (a) in row (n-1) will not be small unless $a_{nn}^{(s)}$ happened to bear some special relationship to the leading principal minor of order (n-1) of A_s, i.e., if the shift was an eigenvalue of this minor. Then no interchange would be necessary in the last step and we would take row (n) - ε/a row (n-1), i.e., R(n) - ε/a R(n-1). The triangular matrix is thus of form (c) above.

When we have post multiplied by all factors except those involving the last two columns, the current matrix will be of form (a) or (b) given below, depending on whether an interchange did or did not occur, i.e., C(n-1,n).

$$
\text{(a)}\quad
\begin{bmatrix}
x & x & x & x & x & x \\
x & x & x & x & x & x \\
 & x & x & x & x & x \\
 & & x & x & x & x \\
 & & & a & 0 & b \\
 & & & & & -b\varepsilon/a
\end{bmatrix}
\qquad
\text{(b)}\quad
\begin{bmatrix}
x & x & x & x & x & x \\
x & x & x & x & x & x \\
 & x & x & x & x & x \\
 & & x & x & x & x \\
 & & & x & a & b \\
 & & & & & -b\varepsilon/a
\end{bmatrix}
$$

To complete the post-multiplication, we add ε/a times column n to column (n-1), no interchange being necessary in general. The final matrix is of form (a) or (b) below.

(a)

$$\begin{bmatrix} x & x & x & x & x & x \\ x & x & x & x & x & x \\ & x & x & x & x & x \\ & & x & x & x & x \\ & & & x & b\varepsilon/a & b \\ & & & & \frac{-b\varepsilon^2}{a^2} & \frac{-b\varepsilon}{a} \end{bmatrix}$$

(b)

$$\begin{bmatrix} x & x & x & x & x & x \\ x & x & x & x & x & x \\ & x & x & x & x & x \\ & & x & x & x & x \\ & & & x & \frac{a+b\varepsilon}{a} & b \\ & & & & \frac{-b\varepsilon^2}{a^2} & \frac{-b\varepsilon}{a} \end{bmatrix}$$

Hence, after restoring the shift, we have

$$a_{nn}^{(s+1)} = a_{nn}^{(s)} - b\varepsilon/a, \qquad a_{n,n-1}^{(s+1)} = -b\varepsilon^2/a^2$$

so that $a_{nn}^{(s+1)}$ is indeed converging and $a_{n,n-1}^{(s+1)}$ is of order ε^2, which we wished to show. Note that any interchange which may take place in the other steps of the reduction are of little significance.

In general, once $a_{n,n-1}^{(s)}$ has become small, it will diminish rapidly in value. When it is negligible to working accuracy we can treat it as zero and the current value of $a_{nn}^{(s)}$ is then an eigenvalue. The remaining eigenvalues are those of the leading principal submatrix of order (n-1). This matrix is itself of Hessenberg form so that we can continue with the same method, working with a matrix of order one less than the original. Since we are expecting all sub-diagonal elements to tend to zero, $a_{n-1,n-2}^{(s)}$ may already be fairly small, and in this case we can immediately use $a^{(s)}_{n-1,n-1}$ as the next value of k_s.

Continuing in this way we may find the eigenvalues one by one, working with matrices of progressively decreasing order. The later stages of the convergence to each eigenvalue will be quadratic generally, and moreover, we can expect that when finding the later eigenvalues in the sequence, we shall have a good start.

CONCLUSION

The basic LR algorithm, although it introduces the basic method of operation, has been seen to be quite tedious and quite possibly inaccurate. However, the introduction of interchanges, reduction to upper Hessenberg form, and shifts of origin have given numerical stability, a reduction of the volume of computation, and accelerated convergence respectively. These modifications have made the LR algorithm a somewhat practical method for the computation of the eigenvalues of a matrix with the restrictions that were placed upon it.

These restrictions, mainly that the matrix have real distinct eigenvalues, are still quite prohibitive. It is generally quite difficult, if not impossible, to determine whether the matrix A has distinct real eigenvalues. There exist, however, more advanced methods which are able to handle matrices with these restrictions. The QR algorithm, which is analogous to the LR technique, is more adaptive to these limitations. For a discussion of the QR algorithm, see Wilkinson (chapter 8, section 28).[3]

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3. See Bibliography

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THE LR ALGORITHM

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The LR algorithm is an iterative method for determining the eigenvalues of a matrix. The basis of the algorithm is the triangularization of a matrix A_1 into the product of a unit lower-triangular matrix L and an upper-triangular matrix R. This yields the equation $A_1 = LR$. Multiplication of these matrices in reverse order yields a matrix similar to A_1, i.e., $RL = A_2$. The algorithm is thus defined by the equations

$$A_{s-1} = L_{s-1}R_{s-1}$$

$$R_{s-1}L_{s-1} = A_s \ .$$

As s approaches infinity, $L_s \to I$ and $R_s \to A_s$. Hence, the desired eigenvalues of A_1 are the diagonal elements of R_s. This is true in general, however, only if the eigenvalues are distinct and real. This orthodox procedure can be numerically unstable and quite slow to converge, unless some modifications are made.

The introduction of Gaussian elimination with interchanges eliminates the problem of numerical instability by assuring that leading principal submatrices of A are non-zero.

The process still requires a large amount of computation. To relieve this problem, the matrix A is reduced to an upper Hessenberg matrix. The upper Hessenberg matrix is invariant with respect to the LR algorithm. This reduces the computation from $(n-1)n^2$ multiplications to n^2 multiplications per step.

The problem of the possible slow rate of convergence of the algorithm is remedied by the use of shifts of origin. By working with the matrix $(A - pI)$, where p is an approximation to λ_i, the rate of convergence can be considerably improved. When the subdiagonal element ($a_{i,i-1}$) is less than 1, choose $p = a_{ii}$.

These modifications definitely improve the practical application of the basic algorithm, however, two major restrictions were assumed in the development. It was assumed that the matrix A had real and distinct eigenvalues. These two limitations are difficult to recognize in most problems, and they require additional methods to handle them. However, if these limitations are not present, the modified LR algorithm will yield the eigenvalues of the matrix A, and the method will be practical to use.