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A.A.Sabir and A.A.Shamin : HOUSEHOLDER'S METHOD FOR THE COMPUTATION OF EIGENVALUES AND EIGENVCTORS FROM THE GIVEN MATRIX AND THEIR APPLICATION TO PRINCIPAL COMPONENT ANALYSIS

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Householder's method for the computation of Eigenvalues and Eigenvectors from the given matrix and their application to Principal Component Analysis.

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Abstract

The Eigenvalue problem has a deceptive simple formulation and background theory has been known for many years, yet the determination of accurate solutions represents a wide variety of challenging problems. A practical treatment of this problem is potentially of great interest to a wide variety of people, including among others are design engineers, theoretical physicists, applied mathematicians and numerical analysts who wish to do research in the matrix field. Though the eigenvalues of a matrix can be determined by QR algorithm with shift of origin and eigenvectors by inverse iterations yet it is recommended to use QR double shift technique in order to calculate eigenvalues and inverse iterations with Hessenberg matrices for the determination of eigenvectors. The reason being that QR double step technique will take only of the order of $5n^2$ multiplications which is very satisfactory result. The best known statistical application of it is that of Principal component analysis.

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1 Introduction

For a number of years it seemed that the Givens process was likely to prove the most efficient method of reducing a matrix to tridiagonal form, but in 1958 Householder's method suggested that this reduction could be performed more efficiently by using the elementary Hermitian orthogonal matrices rather than plane rotations.Moreover the total number of operations is of the order of $2/3n^3$,compared with $4/3n^3$ for Givens method. Further this method requires (n-2) square roots as compared with (n-2)(n-1)/2 for Givens method. For finding out the eigenvalues and eigenvectors procedure as follows.

2 Computational procedure

The main computer program is written by using subroutine EIGENP which is self composed of four subroutines SCALE, HESQR, REALVE and COMVE. Detail is as follows.

EIGENP(N,NM,A,T,EVR,EVI,VECR,VECI,INDIC)

This subroutine finds all the eigenvalues and the eigenvectors of the matrix of order r. First of all the matrix is scaled by SCALE subroutine so that the corresponding rows and columns are approximately balanced and then the matrix is normalised so that the value of the Euclidean norm of the matrix is equal to one. The eigenvalues are computed by QR double step method in the subroutine HESQR. With the help of subroutine REALVE real eigenvectors are determined while complex eigenvectors are computed by the subroutine COMVE. In this subroutine N stands for the order oo the matrix while NM defines the dimension of the two dimensional arrays A, VECR, VECI and the dimension of the one dimensional arrays EVR, EVI and INDIC. Therefore the calling program should contain the following declarations.

DIMENSION A(NM,NN),VECR(NM,NN),VECI(NM,NN),EVR(NM),EVI(NM),INDIC(NM)

Where NM and NN are any numbers equal to or greater than N. The real parameter T must be set equal to the number of binary digits in the mantissa of a single precision floating point number. The real parts of the r computed eigenvalues will be found in the first r places of the array EVI. The components of the normalised eigenvector i corresponding to the eigenvalue stored in EVR(I) and EVI(I) will be found in the first r places of the column i of the two dimensional array VECR and the imaginary components in the first r places of the column i of the two dimensional array VECI.

The real eigenvector is normalised so that the sum of the squares of the components is equal to one. The complex eigenvector is normalised so that the component with the largest value in modulus has its real part equal to one and the imaginary part equal to zero.

The array INDIC indicates the success of the subroutine EIGENP as follows.

Value of INDIC(I)	Eigenvalue(I)	Eigenvector(I)
0	not found	not found
1	found	not found
2	found	found

SCALE(N,M,A,H,PRFACT,ENORM)

This subroutine stores the matrix of the order N from array A into the array H. After words the matrix in the array A is scaled so that the quotient of the absolute sum of the off diagonal elements of column 1 and the absolute sum of the off diagonal elements of row 1 lies within the values of the bound 1 and bound 2. The component of 1 of the eigenvector obtained by using the scaled matrix must be divided by the value found in the PRFACT(1) of the array PRFACT. In this way eigenvector of the non scaled matrix is obtained. After scaling the matrix it is normalised so that the value of the Euclidean norm is equal to one. If the process of the scaling was not successful then the original matrix from the array H would be stored back into A and the eigenvalue problem would be solved by using this matrix. In the above subroutine NM defines the first dimension of the arrays A and H and it must be greater or equal to N. The eigenvalues of the normalised matrix must be multiplied by the scalar ENORM in order that they become the eigenvalues of the non normalised matrix.

HESQR(N,NM,A,H,EVR,EVI,SUBDIA,INDIC,EPS,EX)

This Subroutine finds all the eigenvalues of a real matrix. The orignal matrix A of order N is reduced to the upper Hessenberg form H by means of similarity transformations. The matrix H is preserved in the upper half of the array H and in the array SUBDIA. The special vectors used in the definition of Householder transformation matrices are stored in the lower part of the array H. In this subroutine NM is the first dimension of the arrays A and H and it must be equal or greater than N. The real parts of the N eigenvalues will be found in the N places of the array EVR and the imaginary parts in the first N places of the array EVI. The array INDIC indicates the success of the routine as follows.

Value of the INDIC(I)	Eigenvalue(I)
0	not found
1	found

EPS is a small positive number that numerically represents zero in the program.

EPS=(Euclidean norm of H).EX,where

$EX = 2^{-T}$

In the above relation T is the number of binary digits in the mantissa of a floating point number.

REALVE(N,NM,M,IVEC,A,VECR,EVR,EVI,IWORK,WORK,INDIC,EPS,EX)

This subroutine finds the real eigenvector of the real upper Hessenberg matrix in the array A,corresponding to the real eigenvalue stored in EVR(IVEC). Here inverse iteration method is used. Note that matrix in A is destroyed by the Subroutine. N indicates the order of the upper Hessenberg matrix while NM defines the first dimension of the two dimensional arrays A and VECR which must be equal or greater than N. The value of M is so choosen such that the last N-M components of the eigenvectors become zero. IVEC gives the position of the eigenvalue in the array EVR for which the corresponding eigenvector is computed. The array EVI would contain the imaginary parts of the n eigenvalues if they existetd. The M components of the computed real eigenvector will be found in the first M places of the column IVEC of the two dimensional array VECR. IWORK and WORK are the working stores used during Gaussian elimination and backword substitution process. The array INDIC indicates the success of the routine as follows.

value of INDIC(I)	Eigenvector(I)
1	not found
2	found

EPS is a small positive numbrer that numerically represents zero in the program.

EPS=(Euclidean norm of A).EX, where

$EX = 2^{-T}$

where T represents the number of binary digits in the mantissa of a floating point number.

COMVE(N,NM,M,IVEC,A,VECR,H,EVR,EVI,INDIC,IWORK,SUBDIA,WORK1,WORK2, WORK,EPS,EX)

This subroutine finds the complex eigenvectors from the upper Hessenberg matrix of order N corresponding to the complex eigenvalue with the real part in EVR(IVEC) and the corresponding imaginary part in EVI(IVEC). The matrix on which the inverse iteration is performed is built up in the array A by using the upper Hessenberg matrix preserved in the upper half of the array H and in the array SUBDIA. NM defines the first dimension of the two dimensional arrays A, VECR and H. Further it must be equal or greater than N. M is the order of the submatrix obtained by a suitable

decomposition of the upper Hessenberg matrix if some subdiagonal elements are equal to zero.

The value of M is choosen so that the last N-M components of the complex eigenvectors are zero. The real parts of the first M components of the computed complex eigenvector will be found in the first M places of the column whose top element is VECR and the corresponding imaginary parts of the first M components of the complex eigenvectors will be found in the first M places of the column whose top element is VECR(1, IVEC-1). The array INDIC indicates the success of the routine as follows.

value of INDIC(I)	Eigenvector(I)
1	not found
2	found

The arrays IWORK, WORK1, WORK2 and WORK are the working stores used during the inverse iteration process. EPS is a small positive number that numerically represents zero in the program.

EPS = (Euclidean norm of H) . EX, where

$EX = 2^{-T}$

Here T represents the number of binary digits in the mantissa of a floating point number.

3 Preliminary Modifications In Order To Improve The Accuracy Of The Computed Results

(i) The matrix is scaled by a sequence of similarity transformations so that the absolute sums of corresponding rows and columns are roughly equal.

(ii) The scaled matrix is normalised so that the value of the Euclidean norm is equal to one. The main part of the process commences with the reduction of the matrix to an upper Hessenberg form by means of similarity transformations. Then the QR double step iterative process is performed on the Hessenberg matrix until all elements of the subdiagonal that converge to zero are in modulus less than $2^{-t}\|H\|_E$, where t is the number of binary digits in the mantissa of a floating point number. The eigenvalues are then extracted from this reduced form. Inverse iterations are performed on the upper Hessenberg matrix until the absolute value of the largest component of the right hand side vector is greater than the bound under consideration. Normally when it is achieved, one more step is performed to obtain the computed eigenvector, but at each step the residuals are computed and if the residuals of the particular step are greater in absolute value then the residuals of the previous step is accepted as the computed eigenvector.

4 Statistical Application

The best known statistical application employing eigenvalue and eigenvector is that of principal component analysis. This method was first developed by Hoteling to deal with problems in psychology but has since been applied in many areas including diverse disciplines. Ingeneral, the method may be appled to reduce the dimensionality of problem in terms of the number of variables to to be analysed. The method is also applied to classify the initial variables into sets such that variables within a given set have certain characteristics in common. Suppose that we have a set ofstatistical variables,

$$X_1, X_2, X_3, ..., X_p \tag{1}$$

and would like to determine a normalised linear combinations of these variables,

$$U_1 = a_{11}X_1 + a_{12}X_2 + ... + a_{1p}X_p, \quad sum_{i=1}^{p} a_{1i}^2 = 1 \tag{2}$$

with maximum variance. We can determine a second normalised linear combination of the variables,

$$U_2 = a_{21}X_1 + a_{22}X_2 + ... + a_{2p}X_p, \quad sum_{i=1}^{p} a_{2i}^2 = 1 \tag{3}$$

With maximum variance which is uncorrelated with the first that is,

$cov(u_1, u_2) = 0$,similarly a third normalised linear combination of maximum variance which is uncorrelated with the first two can be determined and so on determination of a_ij affords a means of reducing the set of original variables (1) to a smaller set,

$$U_1, U_2, U_3, ..., U_k, \quad k < p \tag{4}$$

where U_i are called principal components. Let us consider that a_{ij} are the population values and the matrix S to be a symmetric matrix of population variances and covariances such that

$$S_{ij} = E[(x_i - u_i)(x_j - u_j)] \tag{5}$$

,

If $\lambda_1, \lambda_2, ...\lambda_i$ are eigenvalues and $X_1, X_2, ..., X_i$ are eigenvectors then,

$$var(U_i) = \lambda_i \tag{6}$$

$$X_i = \begin{pmatrix} a_{i1} \\ a_{i2} \\ a_{i3} \\ \vdots \\ a_{ii} \end{pmatrix} \tag{7}$$

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