ADDIS ABABA UNIVERSITY

SCHOOL OF GRADUATE STUDIES

DEPARTMENT OF MATHEMATICS

GRADUATE SEMINAR REPORT

ON

FINDING EIGENVALUES BY QR METHOD

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Content

CHAPTER ONE

Introduction

1.1 Basic terminologies

Let A be an $n \times n$ real matrix.

- A is non singular if $|A| \neq 0$. Otherwise A is singular.
- Transpose of a matrix A or a vector X is its reflection along the main diagonal. It is denoted by A^T *or* X^T.
- A is null matrix if $a_{ij} = 0 \; for \; i, j = 1(1)n$.
- A is unit matrix if $a_{ij} = 0 \; for \; i \neq j \; , a_{ij} = 1 \; for \; i = j, \; i, j = 1(1)n$.
- A is involuntary if $A^2 = I$.
- A is symmetric if it satisfies the property, $A^T = A$. This implies the i^{th} column and the i^{th} row of the matrix are identical for all i ,$1 \leq i \leq n$.
- A is orthogonal if it satisfies $A^T = A^{-1} \; or \; A^T A = I = AA^T$.
- A set $\{w_i\}$,$i = 1,2,3,..., n$, of non zero vectors are orthogonal if

  $w_i^T w_i = 0 \;\; when \;\; i \neq j, \;\; and \;\; w_i^T w_i \neq 0 \;\; when \;\; i = j$. More over, if $w_i^T w_i = 1$, the set of vectors, w_i are said to be orthonormal.
- an $n \times n$ matrix A is said to be Hermitian matrix if A is equal to its conjugate transpose $\left(A = A^H\right)$.i.e. $A = \left(a_{ij}\right) \Rightarrow a_{ij} = \bar{a}_{ij} \;\; or \;\; equivalently \;\; A^H A = I = AA^H$

Note: In real case it is analogous to symmetric matrix.

- A is unitary if $A^H A = I = AA^H$.
- A is diagonal matrix if $a_{ij} = 0, for \; i \neq j$
- A is lower triangular if $a_{ij} = 0 \; , for \; j > i$
- A is upper triangular if $a_{ij} = 0 \; , for \; i > j$
- A is tridiagonal if $a_{ij} = 0 \; , for \; |i - j| > 1$.

- A is said to be diagonally dominant if $|a_{ii}| \geq \sum_{\substack{j=1 \\ i \neq j}}^{n} |a_{ij}|$
- A is said to be Hessenberg matrix if the entries for $|i-j| > 1$ are all zero.
- A is upper Hessenberg if the entries for $i - j > 1$ are all zero.
- A is lower Hessenberg if the entries for $j - i > 1$ are all zero.

Illustration:

A 5×5 Hessenberg matrix is indicated by:

$$\begin{bmatrix} * & * & * & * & * \\ * & * & * & * & * \\ 0 & * & * & * & * \\ 0 & 0 & * & * & * \\ 0 & 0 & 0 & * & * \end{bmatrix} = upper\ \ Hessenberg\ \ \ matrix.$$

$$\begin{bmatrix} * & * & 0 & 0 & 0 \\ * & * & * & 0 & 0 \\ * & * & * & * & 0 \\ * & * & * & * & * \\ * & * & * & * & * \end{bmatrix} = lower\ \ Hessenberg\ \ \ matrix.$$

- A is a permutation matrix if it has precisely one entry whose value is one in each column and row, and all of whose other entries are zero.

$$A = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} \ a3 \times 3\ \ permutation\ \ matrix..$$

- A is said to be positive definite matrix, if

  $x^{*}Ax > 0\ \ for\ \ any\ \ vector\ \ x \neq 0\ \ and\ \ x^{*} = \left(\bar{x}\right)^{T}$. Further, $x^{*}Ax = 0\ \ iff\ \ x = 0.$

  If A is a Hermitian, strictly diagonal dominant matrix with positive real diagonal entries, then A is positive definite.

Positive definite matrices have the following important properties.

i. If A is non singular and positive definite, then $B = A^{*}A$ is Hermitian and positive definite.

ii. The eigenvalue of a positive definite matrix are all positive.

iii. All the leading minors of A are positive.

Definition: A matrix norm, $\|A\|$, is a non negative number which satisfies the properties:

$i)\quad \|A\| > 0,\ if\ \ A \neq 0 \quad and\ \ \|0\| = 0$

$ii)\quad \|cA\| = |c|\|A\| \ \ for\ \ an\ arbitrary\ complex\ \ number\ c.$

$iii)\ \ \|A + B\| \leq \|A\| + \|B\|$

$iv)\ \ \|AB\| \leq \|A\|\|B\|$

The most known norms are:

i. Frobenius or Euclidean norm

$$F(A) = \left(\sum_{i,j=1}^{n} |a_{ij}|^{2} \right)^{\frac{1}{2}}$$

ii. Maximum norm

$$\|A\| = \|A\|_{\infty} = \max_{i} \sum_{k} |a_{ik}| \quad (\max imum\ \ absolute\ row\ sum)$$

$$\|A\| = \|A\|_{1} = \max_{k} \sum_{i} |a_{ik}| \quad (\max imum\ \ absolute\ column\ sum)$$

iii. Hilbert norm or spectral norm

$$\|A\|_{2} = \sqrt{\lambda}\ ,\ where\ \ \lambda = \rho(A^{*}A)$$

If A is Hermitian or real and symmetric, then

$\lambda = \rho(A^{2}) = \rho^{2}(A) \ \ so\ \ that\ \ \|A\|_{2} = \rho(A)$

Definition: The quantity $k(A) = \|A^{-1}\|\|A\|$ is called the condition number of the matrix A and is denoted by cond (A).

- If k (A) is large, the system of equations $AX = b$ is said to be ill-conditioned.
- If k (A) is near unity, the system is said to be well conditioned.

1.2 Eigenvalues and Eigenvectors

Consider a system of n linear algebraic equations in n unknowns:

$$
\begin{aligned}
a_{11}x_1 + a_{12}x_2 + \ldots + a_{1n}x_n &= b_1 \\
a_{21}x_1 + a_{22}x_2 + \ldots + a_{2n}x_n &= b_2 \qquad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(1) \\
&\vdots \\
a_{n1}x_1 + a_{n2}x_2 + \ldots + a_{nn}x_n &= b_n
\end{aligned}
$$

Where $a_{ij}\ ,(i,j = 1(1)n)$ are the known coefficients

$b_i\ ,(i = 1(1)n)$ are the known constants and

$x_i\ ,(i = 1(1)n)$ are the unknowns to be determined.

If all the b_i 's are zero then the system of equation (1) is said to be Homogenous, and if at least one of b_i is not zero then it is said to be in-Homogenous.

In matrix notation we can rewrite (1) as

$$Ax = b \qquad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(2)$$

The system (2), $(b = 0)$ & $\det(A) \neq 0$ may then be written as $Ax = \lambda x\ ,(A - \lambda I)x = 0$, where I is $n \times n$ identity matrix.

To have a non-trivial solution $x \neq 0$, the determinant of the matrix $(A - \lambda I)$ must be zero,

i.e. $\det(A - \lambda I) = 0 \quad \ldots\ldots\ldots(3)$

The equation (3) is called characteristic equation.

The n roots $\lambda_1, \lambda_2, \ldots, \lambda_n$ are called the eigenvalues of A and may be distinct or repeated, real or complex. Corresponding to each eigenvalue λ_i , there exist an eigenvector x_i which is a non-trivial solution of $(A - \lambda_i I)x_i = 0$.

Example: Find all the eigenvalues and the corresponding eigenvectors of:

$$A = \begin{bmatrix} 1 & 2 & -2 \\ 1 & 1 & 1 \\ 1 & 3 & -1 \end{bmatrix}$$

Solution:

$$\det(A-\lambda I)=\begin{vmatrix}1-\lambda & 2 & -2\\ 1 & 1-\lambda & 1\\ 1 & 3 & -1-\lambda\end{vmatrix}=-\lambda^3+\lambda^2+4\lambda-4$$ There fore, the eigenvalues are the solution of the characteristic equation

$-\lambda^3+\lambda^2+4\lambda-4=0\ \ these\ \ are\ \lambda_1=1\ ,\ \lambda_2=2\ \&\ \lambda_3=-2$

The eigenvectors corresponding to each eigenvalues are:

$$For\ \lambda_1=1,(A-I)x=\begin{bmatrix}0 & 2 & -2\\ 1 & 0 & 1\\ 1 & 3 & -2\end{bmatrix}x=0.$$

$$the\ \ solution\ is\ x=\begin{bmatrix}-1\\ 1\\ 1\end{bmatrix}$$

$$For\ \lambda_2=2,\ \ (A-2I)x=\begin{bmatrix}-1 & 2 & -2\\ 1 & -1 & 1\\ 1 & 3 & -3\end{bmatrix}x=0.$$

$$the\ \ solution\ is\ x=\begin{bmatrix}0\\ 1\\ 1\end{bmatrix}$$

$$For\ \lambda_2=-2,\ (A+2I)x=\begin{bmatrix}3 & 2 & -2\\ 1 & 3 & 1\\ 1 & 3 & 1\end{bmatrix}x=0.$$

$$the\ \ solution\ is\ x=\begin{bmatrix}8\\ -5\\ 7\end{bmatrix}$$

1.3 Properties of Eigen problems

- Given $Ax_i=\lambda_i x_i$ ....(1)

  Multiplying equation (1) by an arbitrary constant c and putting $y_i=cx_i, we\ \ get\ \ Ay_i=\lambda_i y_i$. This shows that cA has the same eigenvalues with A but different eigenvectors.

- Pre multiplying $Ax=\lambda x$, m times by A we obtain $A^m x=\lambda^m x.$ From this we conclude that λ^m is an eigenvalues of A^m and has the same eigenvectors with A.

Substituting $A^m x = \lambda^m x.$ in to

$$p(\lambda) = (-1)^n \lambda^n + a_1 \lambda^{n-1} + \ldots + a_n = 0, we \ \ get \ \ p(A) = 0$$

Which gives the result that, a square matrix A satisfies its own characteristic equation.

- Suppose that the matrix A has eigenvalues λ_i with eigenvectors u_i and that A has an inverse A^{-1}. Then $Au_i = \lambda_i u_i$ which may be written as $A^{-1}u_i = \frac{1}{\lambda_i}u_i$. This shows that the inverse matrix A^{-1} has the same eigenvectors as A but has the eigenvalues $\frac{1}{\lambda_i}$.
- Replacing the matrix A in $\det(A - \lambda I) = 0$ by the transpose matrix A^T we get $\det(A^T - \lambda I) = \det(A - \lambda I) = 0$. Thus A and A^T have the same eigenvalues.
- Triangular matrices have their eigenvalues on the diagonal of the matrix.

To illustrate this idea, consider the upper triangular matrix U:

$$U = \begin{bmatrix} u_{11} & u_{12} & u_{13} & \cdots & u_{1n} \\ 0 & u_{22} & u_{23} & \cdots & u_{2n} \\ 0 & 0 & u_{33} & \cdots & u_{3n} \\ - & - & - & - & - \\ 0 & 0 & 0 & \cdots & u_{nn} \end{bmatrix}$$

The Eigen problem $(U - \lambda I)$ is given by:

$$U = \begin{bmatrix} (u_{11} - \lambda) & u_{12} & u_{13} & \cdots & u_{1n} \\ 0 & (u_{22} - \lambda) & u_{23} & \cdots & u_{2n} \\ 0 & 0 & (u_{33} - \lambda) & \cdots & u_{3n} \\ - & - & - & - & - \\ 0 & 0 & 0 & \cdots & (u_{nn} - \lambda) \end{bmatrix}$$

The characteristic polynomial, $|U - \lambda I|$ yields

$$(u_{11} - \lambda)(u_{22} - \lambda)(u_{33} - \lambda) \ . \ . \ . \ (u_{nn} - \lambda) = 0 \quad \ldots\ldots\ldots\ldots(*)$$

The roots of (*) are the eigenvalue of matrix U. Thus, $\lambda_i = u_{ii}$,$(i = 1,2,\ldots,n)$

1.4 Bounds on Eigenvalues

The bounds on the Eigenvalue of the matrix A are given by the following theorem.

Gerschgorin Theorem The largest eigenvalue in modulus of a square matrix A can not exceed the largest sum of the moduli of the elements along any row or any column.

Proof: Let λ_i be an eigenvalue of A and x_i be the corresponding eigenvector. Then we have $Ax_i = \lambda_i x_i$

$$a_{11}x_{i,1} + a_{12}x_{i,2} + \ldots + a_{1n}x_{i,n} = \lambda_i x_{i,1}$$
$$a_{21}x_{i,1} + a_{22}x_{i,2} + \ldots + a_{2n}x_{i,n} = \lambda_i x_{i,2}$$

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$$a_{n,1}x_{i,1} + a_{n2}x_{i,2} + \ldots + a_{nn}x_{i,n} = \lambda_i x_{i,n}.$$

Let $\left|x_{i,k}\right| = \max_r \left|x_{i,r}\right|$. Select the k^{th} equation and divide it by $x_{i,k}$ .We get

$$\lambda_i = a_{k1}\frac{(x_{i,1})}{(x_{i,k})} + a_{k2}\frac{(x_{i,2})}{(x_{i,k})} + \ldots + a_{kk} + \ldots + a_{kn}\frac{(x_{i,n})}{(x_{i,k})}$$

And $|\lambda_i| \le |a_{k1}| + |a_{k2}| + \ldots |a_{kk}| + \ldots + |a_{kn}|$

Because $\left|\frac{x_{i,j}}{x_{i,k}}\right| \le 1$, $j = 1(1)n.$

Since k is arbitrary, we get $|\lambda| \le \max_i \sum_{j=1}^{n} |a_{ij}|$

Since the eigenvalues of A^T *are* the same as those of A, the theorem is also true for columns.

Brauer Theorem Let p_k be the sum of the moduli of the elements along the k^{th} row excluding the diagonal element a_{kk} .Then, every eigenvalues of A lies inside or on the boundary of at least one of the circles $|\lambda - a_{kk}| = p_k$, k=1(1)n.

Proof: From the above theorem we have

$$\lambda_i - a_{kk} = a_{k1}\left(\frac{x_{i,1}}{x_{i,k}}\right) + a_{k2}\left(\frac{x_{i,2}}{x_{i,k}}\right) + \ldots + a_{kn}\left(\frac{x_{i,n}}{x_{i,k}}\right)$$

There fore, all the eigenvalues of A lie inside or on the union of the above circles. Again, since A and A^T have the same eigenvalues, we find that all the eigenvalues lie in the union of the n circles $|\lambda_i - a_{kk}| \le \sum_{\substack{j=1 \\ j\ne k}}^{n} |a_{jk}|$, $k = 1(1)n.$

The bounds obtained here are all independent .Hence; all the eigenvalues of A must lie in the intersection of these bounds. These circles are called the Gerschgorin circles and the bounds are called the Gerschgorin bounds.

If A is a real symmetric matrix, then we obtain an interval which contains all the eigenvalues of A.

Example: using the above theorems estimate the eigenvalues of a matrix

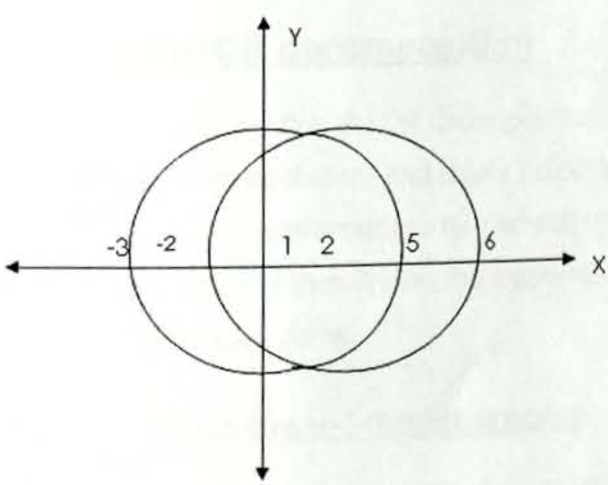
$$A = \begin{bmatrix} 1 & 1 & 1 \\ 2 & 1 & 2 \\ 1 & 3 & 2 \end{bmatrix}$$

The eigenvalues lie in the regions

- $|\lambda| \le 6$, $|\lambda| \le 5$
- The union of the circles

$|\lambda - 1| \le 3$, $|\lambda - 1| \le 4$, $|\lambda - 2| \le 3$

The first union gives $|\lambda - 1| \le 4$ *and* $|\lambda - 2| \le 4$ and the second union gives $|\lambda - 1| \le 4$. the intersection of these circles gives the bound of eigenvalues.



The true eigenvalues are $\lambda = \{\ 4.791288,\ \ -1,\ \ \ 0.208712\ \}$

CHAPTER TWO

The QR method

It is not easy to calculate eigenvalues for most matrices; characteristic polynomials are difficult to compute. Even if we know the characteristic polynomial, most methods for finding zeros can not be depended up on to produce all the zeros with reasonable speed and accuracy. For this and others numerical analysts have found an entirely different way to calculate eigenvalues of a matrix A. the one which is QR method of finding eigenvalues. This is the most efficient and widely used general method for the computation of all the eigenvalues of a general (symmetric and non-symmetric) matrix, using the fact that any matrix similar to A has the same eigenvalues. The idea is by factorizing A=QR where Q is orthogonal and R is upper triangular matrix, create a sequence of matrices similar to A which converges to upper triangular matrix; if this can be done then the diagonal entries of the limit matrix are the eigenvalues of A.

The remarkable discoveries are that the method can be done with great accuracy and it will converge for almost all matrices. Because, the method of orthogonal triangularization is analogous to Gaussian elimination the condition or stability of eigenvalues of a general real matrix A will not be worsen/changed.

NOTE: Assume all the matrices on this paper are real matrices.

2.1 Computing the QR decomposition

There are several methods for actually computing the QR decomposition, such as by means of the Gram-Schmidt process, Givens rotations and House holder transformations. Even though, this paper uses householder transformations for Computing the QR decomposition to establish the algorithms and then finding the eigenvalues through out the page, each of the methods are discussed below.

2.1.1 Using the Gram-Schmidt process

Consider the Gram-Schmidt process applied to the columns of the matrix $A = \lfloor a_1 , a_2 ,........, a_n \rfloor$, with inner product $\langle v, w \rangle = v^T w$

Define the projection:

$$\Pr oj_{e}^{a} = \frac{\langle e,a\rangle}{\langle e,e\rangle} a$$

$$Then: U_1 = a_1 \qquad e_1 = \frac{U_1}{\|U_1\|}$$

$$U_2 = a_2 - \Pr oj_{e_1}^{a_2} \qquad e_2 = \frac{U_2}{\|U_2\|}$$

$$U_3 = a_3 - \Pr oj_{e_1}^{a_3} - \Pr oj_{e_2}^{a_3} \qquad e_3 = \frac{U_3}{\|U_3\|}$$

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$$U_k = a_k - \sum_{j=1}^{k-1} \Pr oj_{e_j}^{a_k} \qquad e_k = \frac{U_k}{\|U_k\|}$$

We then rearrange the equations above so that the a_i's are on the left, using the fact that the e_i's are unit vectors:

$$a_1 = \langle e_1, a_1\rangle e_1$$

$$a_2 = \langle e_1, a_2\rangle e_1 + \langle e_2, a_2\rangle e_2$$

$$a_3 = \langle e_1, a_3\rangle e_1 + \langle e_2, a_3\rangle e_2 + \langle e_3, a_3\rangle e_3$$

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$$a_k = \sum_{j=1}^{k} \langle e_j, a_k\rangle e_j$$

$$where\ \langle e_i, a_i\rangle = \|U_i\|$$

This can be written in matrix form: $A = QR$

$$Where\ Q = [e_1, e_2, \ldots\ldots, e_n]\ and\ R = \begin{bmatrix} \langle e_1,a_1\rangle & \langle e_1,a_2\rangle & \langle e_1,a_3\rangle & \ldots\ldots \\ 0 & \langle e_2,a_2\rangle & \langle e_2,a_3\rangle & \ldots\ldots \\ 0 & 0 & \langle e_3,a_3\rangle & \ldots\ldots \\ . & . & . & \\ . & . & . & \\ . & . & . & \end{bmatrix}$$

Example: Consider the decomposition of

$$A = \begin{bmatrix} 12 & -51 & 4 \\ 6 & 167 & -68 \\ -4 & 24 & -41 \end{bmatrix}$$

Recall that an orthogonal matrix Q has the property $QQ^T = I$. Then, we can calculate Q by means of Gram-Schmidt as follows:

$$U = (U_1 \quad U_2 \quad U_3) = \begin{bmatrix} 12 & -69 & -\frac{58}{5} \\ 6 & 158 & \frac{6}{5} \\ -4 & 30 & -33 \end{bmatrix}$$

$$Q = \begin{pmatrix} \frac{U_1}{\|U_1\|} & \frac{U_2}{\|U_2\|} & \frac{U_3}{\|U_3\|} \end{pmatrix} = \begin{bmatrix} \frac{6}{7} & -\frac{69}{175} & -\frac{58}{175} \\ \frac{3}{7} & \frac{158}{175} & \frac{6}{175} \\ -\frac{2}{7} & \frac{6}{35} & -\frac{33}{35} \end{bmatrix}$$

Thus, we have $A = QQ^T A = QR$

$$R = Q^T A = \begin{bmatrix} 14 & 21 & -14 \\ 0 & 175 & -70 \\ 0 & 0 & 35 \end{bmatrix}$$

2.1.2 Using Givens Rotations

QR decompositions can also be computed with a series of Givens rotations. Each rotation makes zeros an element in the sub diagonal of the matrix, forming the R matrix. The concatenation of all the Givens rotations forms the orthogonal Q matrix.

In practice, Givens rotations are not actually performed by building a whole matrix and doing a matrix multiplication. A Givens rotation procedure is used instead which does the equivalent of the sparse Givens matrix multiplication, with out the extra work of handling the sparse elements, Givens rotations procedure is useful in situations where only relatively few off diagonal elements need to be zeroed, and is more easily parallelized than House holder transformations.

Example: Let us calculate the decomposition of

$$A = \begin{bmatrix} 12 & -51 & 4 \\ 6 & 167 & -68 \\ -4 & 24 & -41 \end{bmatrix}$$

First, we need to form a rotation matrix that makes zero the lower most left element, $a_{31} = -4$ .We form this matrix using the Givens rotation method, and call the matrix G_1.We will first rotate the vector $(6\ ,-4)$,to point along the x-axis: this vector has an angle $\theta = \arctan\left(\frac{-4}{6}\right)$.We create the orthogonal Givens rotation matrix, G_1 :

$$G_1 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos\theta & \sin\theta \\ 0 & -\sin\theta & \cos\theta \end{bmatrix} \approx \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0.83205 & -0.55470 \\ 0 & 0.55470 & 0.83205 \end{bmatrix}$$

And the result of $G_1 A$ now has a zero in the a_{31} element.

$$G_1 A \approx \begin{bmatrix} 12 & -51 & 4 \\ 7.21110 & 125.6396 & -33.83671 \\ 0 & 112.6041 & -71.83368 \end{bmatrix}$$

We can similarly form Givens matrices G_2 *and* G_3, which will zero the sub diagonal elements a_{21} *and* a_{32} forming a triangular matrix R. The orthogonal matrix Q^T is formed from the concatenation of all the Givens matrices $Q^T = G_3 G_2 G_1$. Thus, we have $G_3 G_2 G_1 A = Q^T A = R$, and the QR decomposition is $A = QR$.

2.1.3 <u>Using House Holder Transformations</u>

<u>Definition</u>: *Let* $w \in \Re^n$ *with* $w^T w = 1$. *The* $n \times n$ *matrix* $P = I - 2ww^T$ is called a House Holder matrix.

Using such a matrix, we can apply House Holder transformations which are used to selectively zero out blocks of entries in vector or columns of matrices in a manner that is extremely stable with respect to round-off errors.

Theorem

A matrix of the form $P = I - 2ww^T$ *with* $w \in \Re^n$, $w^T w = 1$, *has the following properties.*

1) $P^T = P$ ....(*P is symmetric*)

2) $P^2 = I$ ....(*P is involutary*)

3) $P^T P = I$ ....(*P is orthogonal*)

4) $P^{-1} = P$ ....(*P is the inverse of itself*)

Proof:

Since $(ww^T)^T = (w^T)^T w^T = ww^T$, *it follows that*

1) $P^T = (I - 2ww^T)^T = I - 2ww^T = P \Rightarrow P$ *is symmetric*

2) $P^2 = (I - 2ww^T)(I - 2ww^T) = I - 2ww^T - 2ww^T + 4w(w^T w)w^T = I,$

since $w^T w = 1 \Rightarrow P$ *is involutary.*

3) *From the property P is symmetric and P is involutary we get*:

$P^T P = PP = P^2 = I \Rightarrow P$ *is orthogonal*

Further since $PP^T = P^T P = I$ *and by uniqueness of inverse* $P^{-1} = P^T = P.$

Lemma: Let $Q \in \Re^{n \times n}$ be an orthogonal matrix. Then the matrix Q^T is also orthogonal and it holds that $\|Qx\|_2 = \|x\|_2 = \|Q^T x\|_2$, $x \in \Re^n$. Thus, Q and Q^T is isometric with respect to Euclidian vector norm.

Proof:

i) $(Q^T)^{-1} = (Q^{-1})^{-1} = Q = (Q^T)^T$ *holds. Thus* Q^T *is also an orthogonal matrix.*

ii) Moreover, the matrix Q is isometric

$$\|Qx\|_2 = (x^T Q^T Qx)^{\frac{1}{2}} = (x^T x)^{\frac{1}{2}} = \|x\|_2.$$

So, the identity $\|Q^T x\|_2 = \|x\|_2$ now follows the statements i & ii

With respect to the Euclidean vector norm $\|\cdot\|_2$, the condition number of a quadratic regular matrix does not change after multiplication with an orthogonal matrix.

Lemma: for orthogonal matrices $Q_1, Q_2 \in \Re^{n \times n}$, $Q_1 Q_2$ is also an orthogonal matrix.

Proof:

We need to show $(Q_1 Q_2)^T (Q_1 Q_2) = I$

$\Rightarrow Q_2^T Q_1^T Q_1 Q_2 = Q_2^T Q_2 = I$

To represent $P = I - 2ww^T$, we need to generate the w's.

For example for the case $n = 3$, we represent

$w = (w_1, w_2, w_3)^T$ *where* $|w_1|^2 + |w_2|^2 + |w_3|^2 = 1$ *and we represent*

$$P = \begin{bmatrix} 1-2|w_1|^2 & -2w_1 \bar{w}_2 & -2w_1 \bar{w}_3 \\ -2 \bar{w}_1 w_2 & 1-2|w_2|^2 & -2w_2 \bar{w}_3 \\ -2 \bar{w}_1 w_2 & -2 \bar{w}_2 w_3 & 1-2|w_3|^2 \end{bmatrix}$$

We usually use w with leading zero components,

$$w = (0, 0, \ldots, w_r, \ldots, w_n)^T = \left(0_{r-1}, \hat{w}^T\right)^T \text{ with } \hat{w} \in C^{n-(r-1)}.$$

$$\textit{Then} \quad P = \left[\begin{array}{ccc} I_{r-1} & . & 0 \\ \hline 0 & . & I_{n-(r-1)-2\hat{w}\hat{w}^T} \end{array}\right]$$

Pre-multiplication and post-multiplication of a matrix A by P will leave the first $r-1$ rows and columns of A respectively unchanged.

House holder matrices will be used to transform a non-zero vector in to any vector containing zeros.

Let $b \neq 0$ be given, $b \in \Re$ and further assume we want to produce P of the form, $P = I - 2ww^T$ such that Pb contains zeros in position $r+1$ through n, for some given $r \geq 1$.

Choose $w = (0, 0, \ldots\ldots, w_r, \ldots\ldots, w_n)^T$ then the first $r-1$ columns of b and Pb are the same.

Let $k = n - (r-1)$, $\quad w = \begin{pmatrix} 0_{r-1} \\ v \end{pmatrix}$, $\; b = \begin{pmatrix} c \\ d \end{pmatrix}$ *with* $C \in \Re^{r-1}, v, d \in \Re^k$. Then our restriction on the form Pb requires the first $r-1$ components of Pb to be C, and

$$\left(I - 2vv^T\right)d = (\alpha, 0, \ldots\ldots 0)^T, \|v\|_2 = 1 \quad \ldots\ldots(1)$$

for some α. From the above property of orthogonal matrices, the length of d is preserved since $I - 2vv^T$ is orthogonal, and thus

$$|\alpha| = \|d\|_2 = s \ \ or \ \alpha = \pm s = \pm\sqrt{d_1^{\ 2} + ... + d_k^{\ 2}} \qquad \text{.......................................}(2)$$

$$Define \ \ R = v^T d$$

$$from \ (1) \ \ d - 2Rv = (\alpha, 0, ...0)^T \qquad \text{.......................................}(3)$$

$$multiplication \ by \ v^T \ and \ use \ of \ \|v\|_2 = 1 \ implies$$

$$R = -\alpha v_1 \text{.......................................}(4)$$

Substituting this in to the first component of (3) gives $d_1 + 2\alpha v_1^{\ 2} = \alpha$

$$\Rightarrow v_1^{\ 2} = \frac{1}{2}\left(1 - \frac{d_1}{\alpha}\right) \qquad \text{.......................................}(5)$$

In order to maximize $v_1^{\ 2}$ and to avoid any possible loss of significance errors in the calculation of v_1, choose the sign of α in (2) by $sign(\alpha) = -sign(d_1)$.

Having v_1, obtain R from (4) return to (3), and using components (2) through m we get

$$v_j = \frac{d_j}{2R}, \ j = 2, 3, ..., m. \qquad \text{.......................................}(6)$$

All these procedure precisely defines w and P. This method has greater numerical stability than the gram-Schmidt and Givens method. As a result, this paper will use House Holder transformation for the decomposition of successive matrices in QR algorithm, through out the page.

The following table gives the number of operations in the k^{th} step of the QR decomposition by House Holder transformation, assuming a square matrix with size n,

Operation	number of operations in the k^{th} step
Multiplications	$2(n-k+1)^2$
Additions	$(n-k+1)^2 + (n-k+1)(n-k) + 2$
Division	1
Square root	1

Summing these numbers over the $(n-1)$ steps reveal $\frac{2}{3}n^3 + n^2 + \frac{1}{3}n - 2 = o(n^3)$.

Using House Holder transformation, for a given real matrix A, we can have $A = QR$ factorization where Q is orthogonal and R is upper triangular. The factorization can be carried out by performing pre-multiplications up on the given matrix A_1 by orthogonal matrices P of the form $I - 2ww^T$ so as to successively reduce the columns of A_1.

Let $P_r = I - 2w^{(r)}w^{(r)T}$, $r = 1, 2, \ldots.$ ....(7)

With $w^{(r)}$ having $r-1$ leading zeros. Writing A in terms of its columns $[A_{\bullet 1}, A_{\bullet 2}, \ldots\ldots, A_{\bullet n}]$

The idea is to first find P_1 *with* $w^{(1)}$ using the above procedure which, when multiplied on the left of A, will produce zeros below the diagonal element a_{11}. That is we get:

$$P_1 \begin{bmatrix} a_{11} & a_{12} & \ldots\ldots a_{1n} \\ a_{21} & a_{22} & \ldots\ldots a_{2n} \\ \ldots & \ldots & \ldots \\ a_{n1} & a_{n2} & \ldots\ldots a_{nn} \end{bmatrix} = \begin{bmatrix} \bar{a}_{11} & \bar{a}_{12} & \ldots\ldots \bar{a}_{1n} \\ 0 & \bar{a}_{22} & \ldots\ldots \bar{a}_{2n} \\ \ldots & \ldots & \ldots \\ 0 & \bar{a}_{n2} & \ldots\ldots \bar{a}_{nn} \end{bmatrix}$$

After this is done, we find P_2 by treating the 2^{nd} column of P_1A as b and multiply P_2 on the left of P_1A produce zeros below the diagonal on 2^{nd} column of P_1A.

$$\textbf{As, } P_2P_1A = P_2 \begin{bmatrix} \bar{a}_{11} & \bar{a}_{12} & \ldots\ldots \bar{a}_{1n} \\ 0 & \bar{a}_{22} & \ldots\ldots \bar{a}_{2n} \\ \ldots & \ldots & \ldots \\ 0 & \bar{a}_{n2} & \ldots\ldots \bar{a}_{nn} \end{bmatrix}$$

$$\Rightarrow p_2 p_1 A = \begin{bmatrix} \bar{a}_{11} & \bar{a}_{12} & \bar{a}_{13} & \ldots\ldots\ldots\ldots \bar{a}_{1n} \\ 0 & \bar{a}_{22} & \bar{a}_{23} & \ldots\ldots\ldots\ldots \bar{a}_{2n} \\ 0 & 0 & \bar{a}_{33} & \ldots\ldots\ldots\ldots \bar{a}_{3n} \\ \ldots\ldots & \ldots\ldots & \ldots\ldots & \ldots\ldots \\ 0 & 0 & \bar{a}_{n3} & \ldots\ldots\ldots\ldots \bar{a}_{nn} \end{bmatrix}$$

Since $w^{(2)}$ contains a zero in position 1, and $P_1 A$ is zero in the first column below position1, the products $P_2 P_1 A$ and $P_1 A$ contain the same elements in row and column 1.

Continue this procedure with each column of A then at a step r of the construction; all elements below the diagonal of column r are zero. So there are $n-1$ House Holder matrices $P_k^{(i)}$ $, k = 1,2,3,...,n-1$ satisfying

$$P_{n-1} P_{n-2} \ldots\ldots P_2 P_1 A = R = (upper \quad triangular \quad matrix) \quad \ldots\ldots(8)$$

To complete the construction, we define the orthogonal matrix $Q^T = P_{n-1} P_{n-2} \ldots\ldots P_2 P_1$ so that $A = QR$ as required.

To evaluate the matrix R of (8) we can use two approaches.

The one is: let

$$A_r = P_r A_{r-1} = \left(I - 2w^{(r)} w^{(r)T} \right) A_{r-1} \quad , r = 1,2,3 \ldots.. \quad \ldots\ldots(9)$$

With $A_0 = A,\ A_{r-1} = R$. If we calculate P_r and then multiply it by A_{r-1} *to form* A_r , the number of multiplications will be $(n-r+1)^3 + \frac{1}{2}(n-r+2)(n-r+1)$.

The other is: rewrite (9) as

$$A_r = A_{r-1} - 2w^{(r)} \left(w^{(r)T} A_{r-1} \right) \quad \ldots\ldots(10)$$

First calculate $w^{(r)}A_{r-1}$; and then calculate $w^{(r)}\left(w^{(r)^T}A_{r-1}\right)$ and A_r. This requires $2(n-(r-1))^2+(n-(r-1))$ multiplications. From this we can see that (10) is a better way to calculate each A_r and finally $R=A_{n-1}$.

After we assure the existence of QR factorization of A it is important to know the uniqueness of the factorization.

Lemma: **(Uniqueness of QR factorization)**

For orthogonal matrices

$Q_1, Q_2 \in \Re^{n\times n}$ *and the upper triangular matrices* $R_1, R_2 \in \Re^{n\times n}$, *Let* $Q_1R_1 = Q_2R_2$ be satisfied. Then there exists a sign matrix s=diag$(\partial_1, \partial_2, ...\partial_n) \in \Re^{n\times n}$ with such $\partial_j \in \{-1,1\}$, such that the following holds:

$$Q_2 = Q_1S \quad R_2 = SR_1$$

Proof:

By assumption, $Q_1^{-1}Q_2 = R_1R_2^{-1} = S$, products and inverses of orthogonal matrices are orthogonal them selves, and the analogous holds for triangular matrices. There for S is an upper triangular matrix as well as orthogonal. i.e.

$$S^{-1} = S\ ,\quad S = \begin{bmatrix} & \cdots\cdots\cdots\cdots & \\ & & \cdots\cdots\cdots \\ & & \cdots\cdots \end{bmatrix} \in \Re^{n\times n}$$

Thus S must be a diagonal matrix,
S= $diag(\partial_1, \partial_2 ....\partial_n) \in \Re^{n\times n}$, and once more, because of $S^{-1} = S^T$ *one obtains* $\partial_j = \dfrac{1}{\partial_j}$ *for* j=1, 2... n, which yields the proposition.

This lemma guaranties that the signs of the diagonal elements of R in A=QR can be Chosen arbitrarily, but the rest of the decomposition is uniquely determined.

Example: Find a QR factorization of

$$A = \begin{bmatrix} 12 & -51 & 4 \\ 6 & 167 & -68 \\ -4 & 24 & -41 \end{bmatrix} u\sin g\ house\ holder\ transformation.$$

Solution:

Take $b=[12\ \ 6\ -4]^T$ and $\alpha=\sqrt{12^2+6^2+(-4)^2}=-14$

The minus sign was chosen since 12>0. Now we set $v_1=\sqrt{\frac{1}{2}\left(1+\frac{12}{14}\right)}=0.963624111$

$R=-\alpha v_1=13.49073756$

$v_2=\frac{d_2}{2R}=0.222374795\ \ ,\ v_3=\frac{d_3}{2R}=-0.148249863$

$$P_1=I-2w_1w_1^T=\begin{bmatrix}-0.85714285460108 & -0.42857142828136 & 0.28571428487849\\ -0.42857142828136 & 0.9010980109742 & 0.06593406578681\\ 0.28571428487849 & 0.06593406578681 & 0.95604395624096\end{bmatrix}$$

$$w_1=\begin{bmatrix}0.963624111\\ 0.222374795\\ -0.148249863\end{bmatrix}$$

$$P_1A=\begin{bmatrix}-0.13999999964415 & -0.21000000101248 & 0.14000000024710\\ 0.00000000004061 & 1.73923076904502 & -0.65692307685009\\ -0.00000000011701 & 0.19384615407377 & -0.42538461539868\end{bmatrix}$$

2^{nd} Transformation

$\alpha=\sqrt{(1.73923076904502)^2+(0.19384615407377)^2}=-1.75$

$v_1=0$

$v_2=\sqrt{\frac{1}{2}\left(1+\frac{1.739230}{1.75}\right)}=0.998460352$

$$v_3=\sqrt{1-v_2^2}=0.055470024\ \ ,w_2=\begin{bmatrix}0\\ 0.998460352\\ 0.055470024\end{bmatrix}$$

$$P_2=I-2w_2w_2^T=\begin{bmatrix}1 & 0 & 0\\ 0 & -0.99384614903193 & -0.11076923937698\\ 0 & -0.11076923937698 & 0.99384615287488\end{bmatrix}$$

$$P_2P_1A=\begin{bmatrix}-0.13999999964415 & -0.21000000101248 & 0.14000000024710\\ -0.00000000002740 & -1.74999999313614 & 0.70000000042805\\ -0.00000000012079 & -0.00000001491235 & -0.34999999395427\end{bmatrix}=R$$

$$Q=(P_2P_1)^T=\begin{bmatrix}-0.85714285460108 & 0.39428570956742 & 0.33142857397732\\ -0.42857142828136 & -0.90285713906881 & -0.03428572225237\\ 0.28571428487849 & -0.17142857921601 & 0.94285714157312\end{bmatrix}$$

From the example just calculated, we see that finding the QR factorization for a 3×3 matrix is tedious by hand. A computer of course is necessary to find QR factorizations and, there fore, to use the QR method for finding eigenvalues.

2.2 The QR Algorithm

In numerical linear algebra, the QR Algorithm is an eigenvalue algorithm: that is, a procedure to calculate the eigenvalues and eigenvectors of a matrix. The key to these methods is the successive factorization of a sequence of matrices $\{A_k\}$, all of which have the same form as the original matrix $A_1 = A_j$.

Definition: Let A and B be two square matrices of same order. If a non singular orthogonal matrix Q can be determined such that $B = Q^{-1}AQ$, then the matrices A & B are said to be similar and the method is called orthogonal similarity transformation. And it has the following properties:

It preserves symmetry form of A

It preserves tridiagonal form of A

It preserves Hessenberg form of A

Theorem: For matrices $A_k, Q_k(Orthogonal), R_k(Uppertriangular)$ satisfy:

$$A_{k+1} = Q_k^T A_k Q_k$$
$$A_{k+1} = (Q_1 Q_2 \ldots\ldots Q_k)^T A_1 (Q_1 Q_2 \ldots\ldots Q_k)$$
$$A^k = (Q_1 Q_2 \ldots\ldots Q_k)(R_k R_{k-1} \ldots\ldots R_1)$$
$$for\ k = 1,2,3,\ldots\ldots$$

Proof:

$$A_k = Q_k R_k, we\ get$$

From $Q_k^T A_k Q_k = R_k Q_k = A_{k+1}$

From the first relation the second identity follows:

$$A_{k+1} = Q_k^T A_k Q_k = Q_k^T Q_{k-1}^T A_{k-1} Q_{k-1} Q_k$$
$$= Q_k^T \ldots Q_1^T A_1 Q_1 Q_2 \ldots Q_k$$

The 3^{rd} identity is obtained through mathematical induction using the following reasoning:

$Q_1Q_2 \ldots Q_kR_kR_{k-1} \ldots R_1 = Q_1Q_2 \ldots Q_{k-1}Q_kR_kR_{k-1} \ldots R_1 = Q_1Q_2 \ldots Q_{k-1}A_kR_{k-1} \ldots R_1$
$\underset{=}{*}\ \underline{\underline{AQ_1Q_2 \ldots Q_{k-1}R_{k-1} \ldots R_2R_1}}\ for\ k \geq 1.$

Where in $(*)$ *the* 2^{nd} identity that was previously shown is used. This completes the proof of the theorem.

From the theorem we can conclude that successive matrices A_k are orthogonally similar to each other.

<u>**Theorem**</u>: Similar matrices have the same eigenvalues.

Proof:
Let λ_i is an eigenvalue of A and u_i is the corresponding eigenvector then
$AU_i = \lambda_i U_i\ or\ Q^T AU_i = \lambda_i Q^T U_i$..(11)
Substituting
$U_i = QV_i\ in\ (11)\ and\ from\ the\ definition\ B = Q^T AQ,\ we\ get\ BV_i = \lambda_i V_i$............................(12)

Thus $Q^T AQ$ has the same eigenvalues as A.

In the basic QR algorithm, sequence of matrices
$A_1, A_2 \ldots A_m\ ,\quad Q_1, Q_2 \ldots Q_m\ ,\ and\ R_1R_2 \ldots R_m$
By this process:
<u>Step 1</u>: Set $A_1 = A\ and\ factorize\ A = QR$
<u>Step 2</u>: First set $A_2 = R_1Q_1;\ then\ factor\ A_2\ as\ A_2 = Q_2R_2$
<u>Step 3</u>: Set $A_3 = R_2Q_2; then\ factor\ A_3\ as\ A_3 = Q_3R_3$

.
.
.
.

At the k^{th} step, a matrix A_k is found, first by using Q_{k-1} *and* R_{k-1} from the previous step; then A_k is factored into Q_kR_k .Thus a QR factorization takes place at each step. We can interrupt the process when the elements below the diagonal if A is non symmetric, the non diagonal elements if A is symmetric are less than a prescribed tolerance. Then the diagonal elements approximate the eigenvalues of A with an error which can be estimated by Gerschgorin's theorem. The eigenvectors are the corresponding columns of multiples of the orthogonal matrices $P_1P_2P_3 \ldots P_{n-1}$.

Example: using QR Algorithm, calculate the eigenvalues of the matrix A= $\begin{bmatrix} 5 & -2 \\ -2 & 8 \end{bmatrix}$

(The true eigenvalues are 4 and 9)

Since each time we need a QR factorization: after step 3, only A_m is listed and the calculated values are rounded.

Step 1: $A_1 = A = \begin{bmatrix} 5 & -2 \\ -2 & 8 \end{bmatrix}$, $\quad Q_1 = Q = \begin{bmatrix} 0.928 & 0.371 \\ 0.371 & 0.928 \end{bmatrix}$

$R_1 = R = \begin{bmatrix} -5.385 & 4.828 \\ 0 & 6.685 \end{bmatrix}$

Step 2: $A_2 = R_1 Q_1 = \begin{bmatrix} 6.793 & -2.482 \\ -2.482 & 6.207 \end{bmatrix}$, $\quad Q_2 = \begin{bmatrix} -0.939 & -0.343 \\ -0.343 & 0.939 \end{bmatrix}$

$R_2 = \begin{bmatrix} -7.233 & -4.462 \\ 0 & 4.977 \end{bmatrix}$

Step 3: $A_3 = R_2 Q_2 = \begin{bmatrix} 8.324 & -1.708 \\ -1.708 & 4.675 \end{bmatrix}$, $\quad Q_3 = \begin{bmatrix} -0.979 & 0.201 \\ 0.201 & 0.979 \end{bmatrix}$

Step 4: $A_4 = \begin{bmatrix} 8.850 & 0.852 \\ 0.852 & 4.149 \end{bmatrix}$

Step 5: $A_5 = \begin{bmatrix} 8.969 & -0.387 \\ -0.387 & 4.030 \end{bmatrix}$

Step 6: $A_6 = \begin{bmatrix} 8.993 & 0.173 \\ 0.173 & 4.006 \end{bmatrix}$

.

.

.

Step 12: $A_{12} = \begin{bmatrix} 8.9999996 & 0.00134 \\ 0.00134 & 4.000018 \end{bmatrix}$

Thus, the approximate eigenvalues are on the diagonal.

Since more iteration is necessary before convergence, this could be quite an expensive task. Fortunately, the work load decreases substantially if we work with Hessenberg or Tridiagonal matrices, which we can do in as much as the QR transformation leaves these forms invariant.

If we count the number of operations involved in a single QR transformation applied to a full matrix, we find that it is of the order of n^3.But the work involved in a single transformation is of the order of n^2 operations for Hessenberg matrices and of n operations for tridiagonal matrices.

Thus the combined algorithm of first reducing a symmetric matrix to tridiagonal form and a non-symmetric matrix to Hessenberg form by House Holder transformations and then applying the QR algorithm is probably the most efficient way to calculate all the eigenvalues of a matrix.

2.3 Reduction of a matrix

Suppose A is real symmetric matrix, then in this method A is reduced to the tridiagonal form by orthogonal transformations representing reflections. The orthogonal transformations are of the form $p = I - 2ww^T$ where w is a column vector, $w \in \Re^n$ such that $w^T w = x_1{}^2 + x_2{}^2 + \ldots + x_n{}^2 = 1$.the vectors w are constructed with the first $(r-1)$ components as zeros, that is: $w_r{}^T = (0, 0, \ldots, 0, x_r, x_{r+1}, \ldots, x_n)$. Since $w_r{}^T w_r = 1 we\ \ have\, x_r{}^2 + x_{r+1}{}^2 + \ldots + x_n{}^2 = 1$.with this choice of w_r form the matrices $p_r = I - 2w_r w_r{}^T$.The similarity transformation is given by $p_r{}^{-1} A p_r = p_r{}^T A p_r = p_r A p_r$. Since p_r is symmetric and orthogonal, we put $A = A_1$ and form successively

$$A_r = P_r A_{r-1} P_r,\ r = 2, 3, \ldots, n-1 \qquad \ldots\ldots (13).$$

At the first transformation, we find $x_r{}'s$ such that we get zeros in the positions $(1, 3), (1, 4), \ldots, (1, n)$ and in the corresponding positions in the first column. There fore, one rotation brings $(n-2)$ zeros in the first row and the first column. In the second rotation, we find x_r's such that we have zeros in $(2, 4), (2, 5), \ldots, (2, n)$ positions. The final matrix is a tridiagonal matrix. The tridiagonalization is completed with exactly n-2 House Holder transformations.

Let us illustrate this procedure using a 4×4 matrix.

$$A = \begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{bmatrix}$$

We note that, since the transformations being used are orthogonal, the sum of the squares of the elements in any row is invariant. Choose

$$w_2^T = [0 \quad x_2 \quad x_3 \quad x_4], \; x_2^2 + x_3^2 + x_4^2 = 1$$

$$p_2 = I - 2w_2w_2^T = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1-2x_2^2 & -2x_2x_3 & -2x_2x_3 \\ 0 & -2x_2x_3 & 1-2x_3^2 & -2x_3x_4 \\ 0 & -2x_2x_4 & -2x_3x_4 & 1-2x_4^2 \end{bmatrix} \quad \ldots\ldots\ldots\ldots(14)$$

Now, the $(1, 3)$ & $(1, 4)$ elements of p_2Ap_2 can become zero only if the corresponding elements in Ap_2 are already zero. The first row of Ap_2 is given by

$$a_{11} \;,\; a_{12} - 2p_1x_2 \;,\; a_{13} - 2p_1x_3 \;,\; a_{14} - 2p_1x_4$$

$$\textit{where } \; p_1 = a_{12}x_2 + a_{13}x_3 + a_{14}x_4 \quad \ldots\ldots\ldots\ldots(15)$$

$$\textit{we now require that} \quad a_{13} - 2p_1x_3 = 0 \quad \ldots\ldots\ldots\ldots(16)$$

$$a_{14} - 2p_1x_4 = 0$$

So that zeros are obtained in the $(1, 3)$, $(1, 4)$ positions. Since the sum of the squares of the elements in any row is invariant under an orthogonal transformation, we have

$$a_{11}^2 + a_{12}^2 + a_{13}^2 + a_{14}^2 = a_{11}^2 + (a_{12} - 2p_1x_2)^2$$

$$\textit{or} \;\; a_{12} - 2p_1x_2 = \pm\sqrt{\{a_{12}^2 + a_{13}^2 + a_{14}^2\}} = \pm s_1 \quad \ldots\ldots\ldots\ldots(17)$$

Notice that s_1 is a known quantity. Multiply

(17) *by* x_2, (16) *by* x_4 *and add. We obtain*:

$a_{12}x_2 + a_{13}x_3 + a_{14}x_4 - 2p_1 = \pm s_1 x_2$

This gives $p_1 = \mp s_1 x_2$

substituting in (17), *we get* $a_{12} \pm 2s_1 x_2^2 = \pm s_1 \pm 2s_1 x_2^2 = \pm s_1 - a_{12}$

$$x_2^2 = \frac{1}{2}\left(1 \mp \frac{a_{12}}{s_1}\right) \qquad (18)$$

This determines x_2.

From (15) & (16) *we have*

$$x_3 = \mp \frac{a_{13}}{(2s_1x_2)} \quad \& \quad x_4 = \mp \frac{a_{14}}{(2s_1x_2)}$$

Usually, we need to find two square roots. One for s_1 and another for x_2. Since x_3 & x_4 contain x_2 in the denominator, we obtain best accuracy if x_2 is large. This can be obtained by taking suitable sign in (18).

Choose $x_2^2 = \frac{1}{2}\left(1 + \frac{a_{12}sign(a_{12})}{s_1}\right)$. The sign of the square root is irrelevant and is taken as plus sign. Hence, $x_3 = \frac{a_{13}sign(a_{12})}{2s_1x_2}$, $x_4 = \frac{a_{14}sign(a_{12})}{2s_1x_2}$. This transformation produces two zeros in the first row and the first column. One more transformation produces zeros in the $(2, 4)$ & $(4, 2)$ positions. The resulting matrix is tridiagonal.

Example: using the House Holders transformation reduce the matrix

$$A = \begin{bmatrix} 4 & -1 & -2 & 2 \\ -1 & 4 & -1 & -2 \\ -2 & -1 & 4 & -1 \\ 2 & -2 & -1 & 4 \end{bmatrix}$$

Solution:

$$w_2 = [0, x_2, x_3, x_4]^T, \; s = \sqrt{a_{12}^2 + a_{13}^2 + a_{14}^2} = 3$$

$$x_2^2 = \frac{1}{2}\left[1 + \frac{(-1)(-1)}{3}\right] = \frac{2}{3}; \quad x_2 = \sqrt{\frac{2}{3}}$$

$$x_3 = \frac{2}{2(3)}\sqrt{\frac{3}{2}} = \frac{1}{\sqrt{6}} \; ; x_4 = -\frac{1}{\sqrt{6}}$$

$$p_2 = I - 2w_2{w_2}^T = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & -\frac{1}{3} & -\frac{2}{3} & \frac{2}{3} \\ 0 & -\frac{2}{3} & \frac{2}{3} & \frac{1}{3} \\ 0 & \frac{2}{3} & \frac{1}{3} & \frac{2}{3} \end{bmatrix}$$

$$A_2 = p_2 A_1 p_2 = \begin{bmatrix} 4 & \frac{1}{3} & 0 & 0 \\ 3 & \frac{16}{3} & \frac{2}{3} & \frac{1}{3} \\ 0 & \frac{2}{3} & \frac{16}{3} & -\frac{1}{3} \\ 0 & \frac{1}{3} & -\frac{1}{3} & \frac{4}{3} \end{bmatrix}$$

2^{nd} $\quad w_3 = [0, 0, x_3, x_4]^T$, $s_1 = \sqrt{{a_{23}}^2 + {a_{24}}^2} = \frac{\sqrt{5}}{3}$

$${x_3}^2 = \frac{1}{2}\left[1 + \frac{\frac{2}{3}}{\frac{\sqrt{5}}{3}}\right] = \frac{1}{2}\left(\frac{\sqrt{5}+2}{\sqrt{5}}\right) = a; \quad x_2 = \sqrt{\frac{2}{3}}$$

$${x_4}^2 = 1 - {x_3}^2 = 1 - \frac{\sqrt{5}+2}{2\sqrt{5}} = \frac{\sqrt{5}-2}{2\sqrt{5}} = \frac{1}{20a} \quad , where\ a = \frac{\sqrt{5}+2}{2\sqrt{5}}$$

$$p_3 = I - 2w_3{w_3}^T = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1-2a & -\frac{1}{\sqrt{5}} \\ 0 & 0 & -\frac{1}{\sqrt{5}} & 1-\frac{1}{10a} \end{bmatrix}$$

$$A_3 = p_3 A_2 p_3 = \begin{bmatrix} 4 & 3 & 0 & 0 \\ 3 & \frac{16}{3} & \frac{-5}{3\sqrt{5}} & 0 \\ 0 & \frac{-5}{3\sqrt{5}} & \frac{16}{3} & \frac{9}{5} \\ 0 & 0 & \frac{9}{5} & \frac{12}{5} \end{bmatrix}$$

If A is non-symmetric, it is reduced to a similar Hessenberg form using the same algorithm. And the transformation to Hessenberg form for non-symmetric case requires $\frac{5}{3}n^3$ operations.

After we prepared the matrix to tridiagonal or Hessenberg, the householder matrices take a simple form when calculating the QR factorization. Having produced $A_1 = Q_1 R_1$ & $A_2 = R_1 Q_1$, we have to know that the form of A_2 is the same as that of A_1 (the QR transformation preserves Hessenberg or tridiagonal form of the original matrix) in order to continue using the less expensive form of QR factorization.

Assume A is Hessenberg form. From section (2.1.3) then the factorization A has the following forms:

$Q = p_1 p_2 \cdots p_{n-1}$ *with each* p_k a House Holder matrix (7) of section (2.1.3)

$$p_k = I - 2w^{(k)} w^{(k)T} \quad , 1 \le k \le n-1 \quad \text{......} (19)$$

Because the matrix A_1 is of Hessenberg form, the vectors $w^{(k)}$ to have the special form

$$w_i^{(k)} = 0 \quad for \quad i < k \quad and \quad i > k+1 \quad \text{......} (20)$$

This can be shown from the equations for the components of $w^{(k)}$ and in particular (12) of section (2.3). From (20), the matrix p_k will differ from the identity is only in the four elements in position $(k\ ,k\ ),\ (k\ ,k+1),(k+1\ ,k\ )$ & $(k+1\ ,k+1)$. And from this it is a fairly straight forward computation to show that Q must be Hessenberg in form. Another important fact is that the product of the tridiagonal and the Hessenberg matrix is again a Hessenberg. Just multiply the two forms of matrices, observing the respective patterns of zeros, in order to prove this idea. Combining these results, observing that R_1 is upper triangular, we have that $A_2 = R_1 Q_1$ must be in Hessenberg form.

For symmetric and tridiagonal case we can show as: If A_1 is symmetric and tridiagonal, then it is trivially Hessenberg. From the preceding result, A_2 must also be Hessenberg. In addition A_2 is symmetric since $A_2^T = \left(Q_1^T A_1 Q_1\right)^T = Q_1^T A_1^T Q_1 = Q_1^T A_1 Q_1 = A_2$ and any symmetric Hessenberg matrix is tridiagonal, we have shown that A_2 is tridiagonal.

<u>Example</u>: using QR algorithm for reduced matrices; find the eigenvalues of the matrix

$$A = \begin{bmatrix} 4 & 2 & 2 & 1 \\ 2 & -3 & 1 & -1 \\ 2 & 1 & 3 & 1 \\ 2 & 1 & 1 & 2 \end{bmatrix}$$

<u>1^{st} Step</u>

Since the original matrix is symmetric, we reduce it to tridiagonal form using section 2.2 and we get the tridiagonal form of:

$$A = \begin{bmatrix} 4 & -3 & 0 & 0 \\ -3 & 2 & 3.16228 & 0 \\ 0 & 3.16228 & -1.4 & -0.2 \\ 0 & 0 & -0.2 & 1.4 \end{bmatrix}$$

<u>2^{nd} Step</u>

Use the subroutine QR method and transform tridiagonal matrix T in to a diagonal matrix.

$$take \quad A_0 = \begin{bmatrix} 4 & -3 & 0 & 0 \\ -3 & 2 & 3.16228 & 0 \\ 0 & 3.16228 & -1.4 & -0.2 \\ 0 & 0 & -0.2 & 1.4 \end{bmatrix},$$

$$A_2 = \begin{bmatrix} 6.16 & 1.90116 & 0 & 0 \\ 1.90116 & -1.713782 & -2.43973 & 0 \\ 0 & -2.43973 & 0.164185 & -0.114069 \\ 0 & 0 & -0.114069 & 1.3896 \end{bmatrix}$$

$$A_3 = \begin{bmatrix} 6.54668 & -0.968456 & 0 & 0 \\ -0.968456 & -3.16916 & 1.37095 & 0 \\ 0 & 1.37095 & 1.2429 & -0.0854415 \\ 0 & 0 & -0.0854415 & 1.37958 \end{bmatrix}$$

.

.

.

$$A_{54} = \begin{bmatrix} 6.64575 & 0 & 0 & 0 \\ 0 & -3.64575 & 0 & 0 \\ 0 & 0 & 1.64575 & 0 \\ 0 & 0 & 0 & 1.35425 \end{bmatrix}$$

Thus the eigen values of A are $\lambda_i = \{6.64575\ , -3.64575\ , 1.64575\ , 1.35425\}$

2.4 Convergence of QR algorithm

Definition: For matrices $A_k = \left(a_{ij}^{(k)}\right)$ & $A = \left(a_{ij}\right) \in \Re^{n\times n}$ one writes $A_k \to A \ \ for\ k \to \infty \Leftrightarrow a_{ij}^{(k)} \to a_{ij} for\ k \to \infty \ (i, j = 1, 2, \ldots, n)$. It is well known that $A_k \to A\ holds\ for\ k \to \infty\ iff\ \|A_k - A\| \to 0\ for\ k \to \infty$ is satisfied for some matrix norm $\|\cdot\| : \Re^{n\times n} \to \Re$.

It is possible to show under certain conditions that the matrices A_k converge to an upper triangular matrix A_∞ with the eigenvalue $\lambda_j\ of\ A$ as diagonal elements $\lambda_j = \left(A_\infty\right)_{jj}$. And the next theorem assures this statement.

Theorem:

Let $A = A_1$ be an $n \times n$ matrix satisfying the following hypotheses.

1) *the eigenvalues λ_i of A have distinict moduli:*

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

2) *the matrix Y with $A = XDY$, $X = Y^{-1}$,*

$D = diag(\lambda_1, \lambda_2, \ldots, \lambda_n) =$ *the Jordan normal form of A,*

has a triangular decomposition.

$$Y = LyRy \ , \ Ly = \begin{bmatrix} 1 & & 0 \\ . & . & \\ . & & . \\ x & \ldots\ldots & 1 \end{bmatrix} \ , \ Ry = \begin{bmatrix} x & \ldots\ldots\ldots & x \\ & . & . \\ & & . \\ 0 & & x \end{bmatrix}$$

Then the matrices A_i, Q_i, R_i of the QR method have the following convergence property:

There are phase matrices

$s_i = diag\left(\sigma_1^{(i)}, \ldots, \sigma_n^{(i)}\right) . \left|\sigma_k^{(i)}\right| = 1$ *such that* $\lim_i s_{i-1}^T Q_i s_i = I$

$$\text{and } \lim_{i\to\infty} s_i^T R_i s_{i-1} = \lim_{i\to\infty} s_{i-1}^T A_i s_{i-1} = \begin{bmatrix} \lambda_1 & x & . & . & . & x \\ & \lambda_2 & & & & . \\ & & & . & & x \\ 0 & & & & & \lambda_n \end{bmatrix}$$

In particular $\lim_{i\to\infty} a_{jj}^{(i)} = \lambda_j$, $j = 1,2,\ldots,n$ *where* $A_i = \left(a_{jk}^{(i)}\right)$

Remark. Hypotheses (2) is used only to ensure that the diagonal elements of A_i Converge to the eigen values λ_j in their natural order, $|\lambda_1| > |\lambda_2| > \ldots > |\lambda_n|$.

Proof:

We carry out the proof under the additional hypotheses $\lambda_n \neq 0$ *so that* D^{-1} exists.

$$\text{Then from } x^{-1} = Y \ , \ A^i = XD^iY$$

$$= Q_x R_x D^i LyRy \quad \ldots\ldots\ldots\ldots (21)$$

$$= Q_x R_x \left(D^i LyD^{-i}\right) D^i Ry$$

Where $Q_x R_x = X$ is a QR decomposition of the nonsingular matrix Q_x and (nonsingular) upper triangular matrix R_x.

Now $D^i LyD^{-i} = \left(l_{jk}^{(i)}\right)$ *is a lower triangular with* $l_{jk}^{(i)} = \left(\frac{\lambda_j}{\lambda_k}\right)^i l_{jk}$, $Ly = (l_{jk})$,

$$l_{jk} = \begin{cases} 1 & \text{for } j = k \\ 0 & \text{for } j < k \end{cases}$$

Since $|\lambda_j| < |\lambda_k|$ *for* $j > k$ *it follows that* $\lim_i l_{jk}^{(i)} = 0$ *for* $j > k$,

and thus $D^i LyD^{-i} = I + E_i$, $\lim_{i\to\infty} E_i = 0$.

Here the speed of convergence depends on the separation of the moduli of the eigenvalue. Next we obtain from (21)

$$\begin{aligned} A^i &= Q_x R_x (I + E_i) D^i Ry \\ &= Q_x (I + R_x E_i R_x^{-1}) R_x D^i Ry \\ &= Q_x (I + F_i) R_x D^i Ry \end{aligned}$$

With $F = R_x E_i R_x^{-1}$, $\lim_i F_i = 0$.*Now the posetive definition matrix* $(I + F_i)^T (I + F_i) = I + H_i$

$H_i = F_i^T + F_i + F_i^T F_i$ *with* $\lim_i H_i = 0$, *has a uniquely determined choleski decomposition.*

$$I + H_i = \tilde{\tilde{R}}_i^T \tilde{\tilde{R}}_i$$

Where $\tilde{\tilde{R}}_i$ is an upper triangular matrix with positive diagonal elements. Clearly, the Choleski factor $\tilde{\tilde{R}}_i$ depends continuously on the matrix $I + H_i$, as is shown by the formulas of the Choleski method. There fore $\lim_i H_i = 0$ implies $\lim_i \tilde{\tilde{R}}_i = I$. Also the matrix

$\tilde{\tilde{Q}} = (I + F_i) \tilde{\tilde{R}}_i^{-1}$ is unitary:

$$\tilde{\tilde{Q}}_i^T \tilde{\tilde{Q}}_i = \tilde{\tilde{R}}_i^{-T} (I + F_i)^T (I + F_i) \tilde{\tilde{R}}_i^{-T} = \tilde{\tilde{R}}_i^{-T} (I + H_i) \tilde{\tilde{R}}_i^{-1} = \tilde{\tilde{R}}_i^{-T} \left(\tilde{\tilde{R}}_i^T \tilde{\tilde{R}}_i \right) \tilde{\tilde{R}}_i^{-1} = I$$

There fore the matrix $I + F_i$ has the QR decomposition $I + F_i = \tilde{\tilde{Q}}_i \tilde{\tilde{R}}_i$,

with $\lim_i \tilde{\tilde{Q}}_i = \lim_i (I + F_i) \tilde{\tilde{R}}_i^{-1} = I, \lim_i \tilde{\tilde{R}}_i = I$

Thus by (6.6.4.14) $A^i = (Q_x \tilde{\tilde{Q}}_i) \left(\tilde{\tilde{R}}_i R_x D^i Ry \right)$ *where* $Q_x \tilde{\tilde{Q}}_i$ *is unitary, and* $\tilde{\tilde{R}}_i R_x D^i Ry$ *is an upper triangular matrix.*

On the other hand, by the theorem on section (2.2), the matrix A^i has the QR decomposition

$A^i = P_i U_i$, $P_i = Q_1 \dots Q_i$, $U_i = R_i \;.\;.\;.\; R_1$. Since the QR decomposition for nonsingular A is unique up to a rescaling of the columns (rows) of Q (respectively R) by phase factors

$\sigma = e^{i\phi}$, there are ph $R_x D R_x^{-1}$ e matrices

$s_i = diag\left(\sigma_1^{(i)},...,\sigma_n^{(i)}\right) \cdot \left|\sigma_k^{(i)}\right| = 1$ With $P_i = Q_x \dot{Q}_i s_i^T$, $U_i = s_i \dot{R}_i R_x D^i Ry$, $i \geq 1$ and it follows that

$$\lim_i P_i s_i = \lim_i Q_x \ddot{Q}_x = Q_x,\; Q_i = P_{i-1}^{-1} P_i = s_{i-1} \dot{Q}_{i-1}^T \dot{Q}_x s_i^T \;,\; \lim_i s_{i-1}^T Q_i s_i = I$$

$$R_i = U_i U_{i-1}^{-1} = s_{i-1} \ddot{R}_i R_x D^i Ry$$

$$Ry^{-1} D^{-i+1} Rx^{-1} \ddot{R}_{i-1}^{-1} s_{i-1}^T = s_i \ddot{R}_i R_x D R_x^{-1} \ddot{R}_{i-1}^{-1} s_{i-1}^T,$$

$$s_i^T R_i s_{i-1} = \ddot{R}_i R_x D R_x^{-1} \ddot{R}_{i-1}^{-1} \;, \lim_i s_i^T R_i s_{i-1} = R_x D R_x^{-1}.$$

$$and \quad finally \;, by \;\; A_i = Q_i R_i \;,\; \lim_i s_{i-1}^T A_i s_{i-1} = \lim_i s_{i-1}^T Q_i s_i s_i^T R_i s_{i-1} = R_x D R_x^{-1}$$

The proof is now complete, since the matrix $R_x D R_x^{-1}$ is upper triangular and has diagonal

D. $R_x D R_x^{-1} = \begin{bmatrix} \lambda_1 & *.........* \\ & \lambda_2.......... \\ & . \quad * \\ 0 & \lambda_n \end{bmatrix}$. Then the diagonal elements of A_{m+1} will converge to the eigenvalues of A ordered from largest to smallest in magnitude. In addition, since $R_x D R_x^{-1}$ is upper triangular, the elements below the diagonal in A_{m+1}, will converge to zero. Generally, if the above hypotheses are satisfied then A_k converges to triangular form for general initial matrix or diagonal form for symmetric initial matrix.

Also it can be seen from the proof that the critical factors in determining the speed of convergence of Q_i, R_i & A_i are the ratio $\dfrac{\lambda_{j+1}}{\lambda_j}$, $1 \leq j \leq n-1$.

In the previous example (section (2.2)) the ratios of successive eigenvalue is $\dfrac{\lambda_2}{\lambda_1} \approx 0.44445$, and if the off-diagonal elements are observed, we see that they decrease with about this ratios.

This implies that the convergence rate depends on the separation between the absolute values of the eigenvalues. And the convergence of QR process is determined by the behavior of the sequence $\{E_k\}$ *where* $E_k = (P_{n-1} P_{n-2} ... P_1)^T$, $\sin ce$ $A_{k+1} = E_k^T A_1 E_k$.

To see that the basic QR method can fail if two different eigenvalues have the same magnitude, try it on the following matrices:

$$A=\begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix} \quad \& \quad B=\begin{bmatrix}3 & -2\\ 4 & -3\end{bmatrix}$$

Each of which has eigenvalue ± 1.
For the case A: Since it is orthogonal, we have

$$A=Q_1R_1 \text{ and } R_1=I \text{ and thus } A_2=R_1Q_1=A$$

And all the iterates $A_k = A.$ *the sequence* $\{A_k\}$ doesn't converge to a diagonal matrix. The same is true for matrix B.

Even, the difference in the magnitudes of the eigenvalues are small, convergence of the QR method can be slow.

Example: Apply QR method to calculate the eigenvalues of the matrix

$$A=\begin{bmatrix}3 & 3\\ 0.333335 & 5\end{bmatrix}$$

Note that the true eigenvalues are 4.001 and 3.999

After computation we find

$$A_{10}=\begin{bmatrix}4.7058 & -3.1764\\ 0.1568 & 3.2941\end{bmatrix}, \quad A_{20}=\begin{bmatrix}4.2582 & -3.3132\\ 0.0201 & 3.7418\end{bmatrix},$$

$$A_{30}=\begin{bmatrix}4.1571 & -3.3259\\ 0.0074 & 3.8428\end{bmatrix}$$

We see that as the theorem guarantees, A_k is converging to an upper triangular matrix and the diagonal elements are heading in the right direction; however, the convergence is very slow. The slowness of convergence is due to the fact that $|\lambda_1| \approx |\lambda_2|$

2.5 QR Algorithm with Shifts

As outlined above QR method works, but convergence is slow, even for matrices of small dimension. This costs money because of the computer time used. But this can be improved by adding a shifting technique that speeds up the rate of convergence. Recall that if λ_j is an eigenvalue of A, then $\lambda_j - S_k$ is an eigenvalue of the matrix B= $A - S_k I$.

The idea is incorporated in the modified step:

$A_k - S_k I = Q_k R_k$ Then form

$$A_{k+1} = R_k Q_k + S_k I, \quad k=1, 2, 3, \ldots \qquad (22)$$

Where $\{S_k\}$ is a sequence whose sum is λ_j.

It is easily seen that A_{k+1} is still similar to A_k.

To illustrate this, $R_k = Q_k^T (A_k - S_k I)$

$$A_{k+1} = S_k I + Q_k^T (A_k - S_k I) Q_k$$

$$= S_k I + Q_k^T A_k Q_k - S_k I$$

$$\Rightarrow A_{k+1} = Q_k^T A_k Q_k \quad , k = 1, 2, 3, \ldots$$

This shows that the eigenvalue of A_{k+1} are the same as those of A_k and the same as those of A.

Here the shift parameter S_k is chosen as a close approximation to some eigenvalue. There are two methods for selecting the parameter S_k.

1) Take $S_k = a_{nn}^{(k)}$
2) By computing eigenvalue of 2×2 sub matrix in lower right corner of the matrix, which is closest to the lower diagonal element $a_{nn}^{(k)}$

More specifically let's consider the reduced tridiagonal matrix to show how we compute the eigenvalues with shift.

$$A_k = \begin{bmatrix} d_1^{(k)} & e_1^{(k)} & 0 \ldots\ldots\ldots 0 \ldots\ldots 0 & & \\ e_1^{(k)} & d_2^{(k)} & e_2^{(k)} \ldots\ldots\ldots 0 \ldots\ldots 0 & & \\ . & & & & \\ . & & & & \\ . & & e_{n-2}^{(k)} & d_{n-1}^{(k)} & e_{n-1}^{(k)} \\ . & & & e_{n-1}^{(k)} & d_n^{(k)} \end{bmatrix}$$

Since $\|A_{k+1}\|_2 = \|Q_k^T A_k Q_k\|_2 = \|A\|_2$. Using the operator matrix norm

The matrices $\{A_k\}$ are uniformly bounded, and consequently the same is true of their elements.

From $e_{n-1}^{(k)} e_{(n-2)}^{(k)} \to 0 \text{ as } k \to \infty$ and the uniform bounded ness of $\{e_{n-1}^{(k)}\} \text{ and } \{e_{n-2}^{(k)}\}$ we have either $e_{n-1}^{(k)} \to 0 \text{ or } e_{n-2}^{(k)} \to 0 \text{ as } k \to \infty$. In the former case, $d_n^{(k)}$ converges to an eigenvalue of A. And in the later case, two eigenvalues can be extracted from the sub matrix $\begin{bmatrix} d_{n-1}^{(k)} & e_{n-1}^{(k)} \\ e_{n-1}^{(k)} & d_n^{(k)} \end{bmatrix}$

Once one or two eigenvalues have been obtained due to $e_{n-1}^{(k)}$ *or* $e_{n-2}^{(k)}$ being essentially zero, the matrix A_k can be reduced in order by one or two rows, respectively. Following this, the QR method with shift can be applied to the reduced matrix.

The choice of shift is designed to make the convergence to zero be more rapid for $e_{n-1}^{(k)}\ e_{n-2}^{(k)}$ than for the remaining off-diagonal elements of the matrix.

With suitably chosen shifts, experimental results show that in the symmetric case fewer than two QR-iterations per eigenvalues are needed.

To illustrate the method with an Example:

Example: Find the eigenvalues of the matrix A= $\begin{bmatrix} 4 & 2 & 2 & 1 \\ 2 & -3 & 1 & 1 \\ 2 & 1 & 3 & 1 \\ 1 & 1 & 1 & 2 \end{bmatrix}$ by using QR method incorporating shifts.

Solution:

First reduce A to its tridiagonal form

$$A_1 = \begin{bmatrix} 4 & -3 & 0 & 0 \\ -3 & 2 & 3.16228 & 0 \\ 0 & 3.16228 & -1.4 & -0.2 \\ 0 & 0 & -0.2 & 1.4 \end{bmatrix}$$

The four elements in the lower right corner are $d_3 = -1.4$, $d_4 = 1.4$ *and* $e_3 = -0.2$ and are used to form the quadratic equation:

$$x^2 - (-1.4 + 1.4)x + (-1.4)(1.4) - (-0.2)(-0.2) = x^2 - 2 = 0$$

Calculation produces the roots $x_1 = -1.41421$ *and* $x_2 = 1.41421$.The roots closest to d_4 is chosen as the first shift $S_1 = 1.41421$, and the first shifted matrix is

$$A_1 - S_1 I = \begin{bmatrix} 2.58579 & -3 & 0 & 0 \\ -3 & 0.58579 & 1.74806 & 0 \\ 0 & 1.74806 & -2.81421 & -1.61421 \\ 0 & 0 & -1.61421 & -0.01421 \end{bmatrix}$$

Next, the factorization $A_1 - S_1 I = Q_1 R_1$ is computed:

$$Q_1 = \begin{bmatrix} -0.65288 & -0.38859 & -0.55535 & 0.33814 \\ 0.75746 & -0.33494 & -0.47867 & 0.29145 \\ 0 & 0.85838 & -0.43818 & 0.26610 \\ 0 & 0 & 0.52006 & 0.85413 \end{bmatrix}$$

$$R_1 = \begin{bmatrix} -3.96059 & 2.40235 & 2.39531 & 0 \\ 0 & 3.68400 & -3.47483 & 0.17168 \\ 0 & 0 & -0.38457 & 0.08024 \\ 0 & 0 & 0 & -0.06550 \end{bmatrix}$$

Then the matrix product is computed in the reverse order to obtain:

$$A_2 = R_1 Q_1 + S_1 I = \begin{bmatrix} 4.40547 & 2.79049 & 0 & 0 \\ 2.79049 & -4.21663 & -0.33011 & 0 \\ 0 & -0.33011 & 0.21024 & -0.03406 \\ 0 & 0 & -0.03406 & -0.05595 \end{bmatrix}$$

The second shift is $S_2 = -0.06024$, the second shifted matrix is $A_2 - S_2 I = Q_2 R_2$, and

$$A_3 = S_2 I + R_2 Q_2 = \begin{bmatrix} 4.55257 & -2.65725 & 0 & 0 \\ -2.65725 & -4.26047 & 0.01911 & 0 \\ 0 & 0.01911 & 0.29171 & 0.00003 \\ 0 & 0 & 0.00003 & 0.00027 \end{bmatrix}$$

The third shift is $S_3 = 0.00027$, the third shifted matrix is $A_3 - S_3 I = Q_3 R_3$, and

$$A_4 = R_3Q_3 + S_3I = \begin{bmatrix} 4.62640 & 2.53033 & 0 & 0 \\ 2.53033 & -4.33489 & -0.00111 & 0 \\ 0 & -0.00111 & 0.29150 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

The first eigenvalue, rounded to five decimal places is given in the calculation

$\lambda_1 = S_1 + S_2 + S_3 = 1.41421 - 0.06023 + 0.00027 = 1.35425$

Next λ_1 is placed in the last diagonal position of A_4 and the process is repeated, but changes are made only in the upper 3×3 corner of the matrix.

$$A_4 = \begin{bmatrix} 4.62640 & 2.53033 & 0 & 0 \\ 2.53033 & -4.33489 & -0.00111 & 0 \\ 0 & -0.00111 & 0.29150 & 0 \\ 0 & 0 & 0 & 1.35425 \end{bmatrix}$$

In a similar manner, one more shift reduces the entry in the second row and third column to zero (to 10 decimal places):

$$S_4 = 0.29150 \quad , \quad A_4 - S_4I = Q_4R_4 \quad , \quad A_5 = R_4Q_4 + S_4I$$

Hence the second eigenvalue is $\lambda_2 = \lambda_1 + S_4$=1.35425+0.29150=1.64575

Finally, λ_2 is placed on the diagonal of A_5 in the third row and column to obtain

$$A_5 = \begin{bmatrix} 4.26081 & -2.65724 & 0 & 0 \\ -2.65724 & -4.55232 & 0 & 0 \\ 0 & 0 & 1.64575 & 0 \\ 0 & 0 & 0 & 1.35425 \end{bmatrix}$$

The final computation requires finding the eigenvalue of the 2×2 matrix in the Upper-left corner of A_5. The characteristic equation is:

$$x^2 - (-4.26081 + 4.55232)x + (4.26081)(-4.55232) - (2.65724)(2.65724) = 0$$

which reduce to $x^2 + 0.29157x - 26.45749$

The roots are $x_1 = 5.00000$ & $x_2 = -5.29150$

And the last two eigenvalues are computed with the calculations

$\lambda_3 = \lambda_2 + x_1 = 1.64575 + 5.00000 = 6064575$ &
$\lambda_4 = \lambda_2 + x_2 = 1.64575 - 5.29150 = -3.64575$
Thus the eigenvalues of A is $\lambda = \{\ 6.64575\ ,\ -3.64575\ ,\ 1.64575\ ,\ 1.35425\ \}$.

2.6 The Double QR Algorithm

As we pointed out earlier, shifting is essential for rapid convergence. A key difference here is that a non-symmetric real matrix can have complex eigenvalues. For example the following matrices have some complex eigenvalues:

$\begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix}$ *and* $\begin{bmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \end{bmatrix}$. This means that good choices for the shifts s_k may be complex, apparently necessitating complex arithmetic. But complex arithmetic can be avoided, however, by a clever trick: seeking an algorithm which produces a real matrix from which the complex eigenvalues can be calculated easily as conjugate roots of 2×2 real principal sub matrices.

Let's see two steps of the generalized QR transformation of a general real matrix A_1.
From the relation $A_{k+1} = P_k I + R_k Q_k \quad k = 1,2,\ldots..$ it follows that

$$A_3 = Q_2^T A_2 Q_2 = Q_2^T Q_1^T A_1 Q_1 Q_2 \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(23)$$

And also

$$\begin{aligned} Q_1 Q_2 R_2 R_1 &= Q_1 (A_2 - P_2 I) R_1 \\ &= (A_1 - P_2 I) Q_1 R_1 \\ &= (A_1 - P_2 I)(A_1 - P_1 I) = T \end{aligned}$$

Thus, setting $Q_0 = Q_1 Q_2$ *and* $R_0 = R_2 R_1$, the formulas above say that $A_3 = Q_0^T A_1 Q_0$ where, by uniqueness, $Q_0 R_0$ is the QR factorization of the non-singular matrix T. It is now clear what should be done. Suppose that P_1 is a complex shifts and that P_2 is forced to be $\bar{P}_1$, then T will be real, Q_0 will be its (real) orthogonal factor, A_3 will be real , and the computation of complex A_2 will be circumvented.

The solution is there fore to use the generalized QR transformation with the proviso that every shift with positive imaginary part is followed by its conjugate, the intermediate complex matrix being avoided as indicated above. Ignoring the storage of the auxiliary matrix T it turns out the formation of T, its decomposition , and the formation of A_3 (one double step) requires at least as much work as two real QR steps. Note that a part from the decided advantage of keeping the arithmetic real there is no extra profit.

Practically, double QR step will result accurate solution for general real matrices. If we use reduction of a matrix and use algorithm with complex shifts reveals a better approximation of eigenvalues.

2.7 Comparison of QR with other iterative methods

The Power algorithm repeatedly multiplies A times a single vector, normalizing after each iteration. The vector converges to an eigenvector of the largest eigenvalue. The methods are based on a one-step procedure. And the power method is very inefficient when all the eigenvalues of a large matrix are desired. And to start iteration the initial vector is needed. More over, power method uses shifts of origin so that we can find the intermediate eigenvalues. On the other hand QR algorithm can be seen as a more sophisticated variation of the basic "power" eigenvalue algorithm, it works with a complete basis of vectors, using QR decomposition to renormalize (and orthogonalize).In QR method we can calculate all the eigenvalues of a general matrix simultaneously based on a two-step procedure. In the first step, the original matrix is transformed to a simpler form that has the same eigenvalues as the original matrix.
In the second step, iterative procedures are used to determine these eigenvalues. For a symmetric matrix A, up on convergence, AQ$\nabla = \nabla Q \wedge$, where $\wedge$ is the diagonal matrix of eigenvalues to which A converged and where Q is a composite of all the orthogonal

similarity transforms required to get there. Unlike power method, in QR method, we can calculate all the eigenvectors as the columns of Q.

Rutishauser method uses almost the same algorithm with QR method. It proposed the LU transformation where L is a lower triangular matrix and U is an upper triangular matrix. In the limit, we get an upper triangular matrix which displays the eigenvalues of A on the leading diagonal. However, QR method replaces L by orthogonal matrix Q and uses the logic: if A is non singular then there exists decomposition A= QR, where Q is orthogonal and R is upper triangular. In LU transformation there are difficulties associated with the practical application of the method ; an arbitrary matrix A_i doesn't always have a factorization $A_i = L_i R_i$ .Even if the decomposition exists, the problem of computing L_i and R_i may be ill conditioned .But QR method is a more modern method which handles these sorts of problems in a uniform way and computes all the eigenvalues and eigenvectors at one time and avoids some of these difficulties. The QR algorithm is also not simple for practical application. It is useful when applied to a matrix in upper Hessenberg form.

Hence, even though the QR algorithm is more expensive than the LU algorithm, its superior numerical properties more than make up for the extra labor.

Givens and House Holder method find the eigenvalues one at a time. And if we want only one eigenvalue, then this algorithm is also appropriate .Even if we want all the eigenvalues, it requires less computation time than the QR algorithm. Givens and House Holder methods are used for only symmetric matrices and it also used for reducing a symmetric matrix into simpler form. And these methods take only a finite number of plane rotations $\frac{(n-1)(n-2)}{2}$ to reduce A to its tridiagonal form in Givens method and in House Holder method (n-2) orthogonal transformations are needed .On the other hand, QR method is used for a general matrix and it uses both Givens and House Holder methods in its step to transform a matrix to its diagonal or Hessenberg form so that it will be easy for calculating the eigenvalues. The common thing for Givens, House Holder and QR method for calculating eigenvalues for symmetric matrices is that they all use two step procedures.

In Givens method one can approximately compute the eigenvalues and by repeated bisections, one can improve these estimates. But in QR method once we calculate the eigenvalues we can not improve the estimates rather we use shifting technique to speed up the convergence.

Jacobi method, like QR method, it is well suited for finding all the eigenvalues and the complete set of orthnormal eigenvectors simultaneously using a series of orthogonal transformations but in Jacobi method the elements that are annihilated by plane rotation may not necessarily remain zero during subsequent transformations and it is applied only on symmetric matrices. However, QR method is widely applicable for arbitrary matrices. For symmetrical matrices the QR algorithm is in fact identical to the Jacobi eigenvalue algorithm. To see this, imagine the QR decomposition computed by Givens rotations. Then the computations are exactly the same in both algorithms.

2.8 Advantage & Disadvantage

Advantage

- QR algorithm is used for arbitrary matrices and finds all the eigenvalues.
- Since a QR factorization can be used to create each new matrix in the sequence, modern implementations of this method are efficient and reliable.
- Each QR factorization can be calculated accurately; it yields easily a new matrix orthogonally similar to the original matrix; and orthogonal similarities tend to minimize the effect of round off errors on the eigenvalues.
- QR algorithm uses shifts to try to speed convergence. And some eigenvalues can be determined early in the iteration, which speeds up the process even more.
- Serious implementations of the QR method save information about each step, which defines the eigenvectors.
- The method offers superior stability properties.

Disadvantage

- The QR method going to have trouble if the matrix has repeated eigenvalues, distinct eigenvalues of the same magnitude or complex eigenvalues.
- It is too laborious
- The transformation to a triangular system by similarity transformations is costier.

2.9 Application of QR method

1) One application of QR decomposition is to find the absolute value of the determinant of a square matrix. Suppose the matrix is decomposed as A=QR.Then we have

det (A) =det (Q).det(R).

Since Q is unitary, $|\det(Q)| = 1$.Thus,

$$|\det(A)| = |\det(R)| = \left|\prod_i r_{ii}\right|,$$

Where r_{ii} are the entries on the diagonal of R.

Further more, because the determinant equals the product of the eigenvalue, we have

$\left|\prod_i r_{ii}\right| = \left|\prod_i \lambda_i\right|$, where λ_i are eigenvalue of A.

2) The other application of QR decomposition is least squares Approximation.

Note: We can extend the QR decomposition for non square, rectangular matrix.

Problem. Suppose the system Ax=b is inconsistent. It is necessary to find such $\bar{x}$ that $\left\|A\bar{x} - b\right\|$ is minimal. Obviously $A\bar{x}$ should be a projection of b onto the image of A.

Theorem: Suppose A is an $m \times n$ matrix, $b \in \Re^m$. Then $Ax = b$ has at least one least Squares solution $\bar{x}$.

1) $\bar{x}$ is a least squares solution of $Ax = b$ if and only if $\bar{x}$ is a solution of the system $A^T A\bar{x} = A^T b$.

2) A has linearly independent columns if and only if $A^T A$ is invertible. In this case the Least squares solution is unique $\bar{x} = \left(A^T A\right)^{-1} A^T b$. Moreover, if $A = QR$ is a QR Factorization of A, then $\bar{x}$ is the only solution of the system $Q^T QRX = RX = Q^T b$ is the least squares solution $\bar{x}$.

Example: Find the least squares solution of the system $AX = \begin{bmatrix} 1 & 1 \\ 2 & -1 \\ -2 & 4 \end{bmatrix} X = \begin{bmatrix} 1 \\ 2 \\ 7 \end{bmatrix}$.

Solution: For QR factorization of A we have $Q = \frac{1}{3}\begin{bmatrix} 1 & 2 \\ 2 & 1 \\ -2 & 2 \end{bmatrix}$, $R = \begin{bmatrix} 3 & -3 \\ 0 & 3 \end{bmatrix}$.

Then $Q^T QRX = Q^T b = \frac{1}{3}\begin{bmatrix} 1 & 2 & -2 \\ 2 & 1 & 2 \end{bmatrix}\begin{bmatrix} 1 \\ 2 \\ 7 \end{bmatrix} = \frac{1}{3}\begin{bmatrix} -9 \\ 18 \end{bmatrix} = \begin{bmatrix} -3 \\ 6 \end{bmatrix}$

$$\Rightarrow 3x_1 - 3x_2 = -3,\ 3x_2 = 6 \Rightarrow X = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 1 \\ 2 \end{bmatrix}$$

Here

$$\|AX - b\| = \left\| \begin{bmatrix} 1 & 1 \\ 2 & -1 \\ -2 & 4 \end{bmatrix}\begin{bmatrix} 1 \\ 2 \end{bmatrix} - \begin{bmatrix} 1 \\ 2 \\ 7 \end{bmatrix} \right\| = \left\| \begin{bmatrix} 3-1 \\ 0-2 \\ 6-7 \end{bmatrix} \right\| = \left\| \begin{bmatrix} 2 \\ -2 \\ -1 \end{bmatrix} \right\| = 3.$$

2.10 Conclusion

In the mathematical subfield of numerical Analysis, Numerical stability is a desirable property of numerical Algorithms. Due to its good numerical stability among other desirable properties, the QR method is generally the method of choice. It is applicable for more general matrices. But in its original form the iterations are relatively expensive. This can be mitigated by first bringing the matrix A to simpler form, with a finite sequence of orthogonal similarity. Iterative methods with shifts are then employed to evaluate the eigenvalues.

Under fairly general conditions the diagonal entries of A_k converge for $k \to \infty$ to the eigenvalues of A which are sorted with respect to their absolute values in decreasing order. But convergence fails if the matrix has repeated eigenvalues, distinct eigenvalues of the same magnitude .In addition a real matrix can have complex eigenvalues and the double QR algorithm is the most suitable method for finding the most accurate eigenvalues for general non symmetric real matrix.

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