Numerical Analysis

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Jacobi Method for Symmetric Matrices

Let A be the given real symmetric matrix. The eigenvalues of A are real and there exists a real orthogonal matrix S such that $S^{-1}AS$ is a diagonal matrix D. The diagonalization is done by applying a series of orthogonal transformations $S_1,\ S_2, \cdots, S_n, \cdots$ as follows.

Among the off-diagonal elements, let $|a_{ik}|$ be the numerically largest element. Then the elements $a_{ih},\ a_{ik},\ a_{kh},\ a_{kk}$ form a 2×2 submatrix A_1 which can be transformed to a diagonal form. We choose

$$S_1^* = \begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix} \tag{1}$$

and find θ such that the 2×2 submatrix A_1 is diagonalized. We have

$$\begin{aligned} S_1^{*-1} A_1 S_1^* &= \begin{bmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{bmatrix} \begin{bmatrix} a_{ii} & a_{ik} \\ a_{ki} & a_{kk} \end{bmatrix} \begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix} \\ &= \begin{bmatrix} a_{ii}\cos^2\theta + 2a_{ik}\sin\theta\cos\theta + a_{kk}\sin^2\theta & (a_{kk} - a_{ii})\sin\theta\cos\theta + a_{ik}\cos 2\theta \\ (a_{kk} - a_{ii})\sin\theta\cos\theta + a_{ik}\cos 2\theta & a_{ii}\sin^2\theta + 2a_{ik}\sin\theta\cos\theta + a_{kk}\cos^2\theta \end{bmatrix} \end{aligned} \tag{2}$$

We now choose θ such that this matrix reduces to a diagonal form. That is, we put

$$\begin{aligned} \frac{1}{2}(a_{kk} - a_{ii})\sin\theta\cos\theta + a_{ik}\cos 2\theta &= 0 \\ \text{or,}\quad \tan 2\theta &= \frac{2a_{ik}}{a_{ii} - a_{kk}}. \end{aligned} \tag{3}$$

This equation produces four values of θ and in order that we may get smallest rotation we require $-\frac{\pi}{4} < \theta < \frac{\pi}{4}$. From (12) we get

$$\theta = \frac{1}{2}\tan^{-1}\left(\frac{2a_{ik}}{a_{ii} - a_{kk}}\right), \quad \text{if} \quad a_{ii} \neq a_{kk} \tag{4}$$

If $a_{ii} = a_{kk}$, then

$$\theta = \begin{cases} \frac{\pi}{4}, & a_{ik} > 0 \\ -\frac{\pi}{4}, & a_{ik} < 0 \end{cases} \tag{5}$$

With the value of θ given in (13), the off-diagonal elements in (26) vanish and the diagonal elements are simplified. The first step is now completed by performing the rotation $S_1^{-1}AS_1$. In the next step the largest off-diagonal element in magnitude in the new rotated matrix is found and the procedure is repeated. We now perform a series of such two dimensional rotations. After finding θ at each step, the rotation is performed with the corresponding orthogonal matrix. For example, if $|a_{ik}|$ is the largest off-diagonal element then we write S_1 as

$$S_1 = \begin{bmatrix} 1 & & & & & & & & \\ & 1 & & & & & & & \\ & & \ddots & & & & & & \\ & & & \cos\theta & \cdots & -\sin\theta & & & \\ & & & \vdots & \ddots & \vdots & & & \\ & & & \sin\theta & \cdots & \cos\theta & & & \\ & & & & & & \ddots & & \\ & & & & & & & 1 & \\ & & & & & & & & 1 \end{bmatrix}$$

where $\cos\theta$, $-\sin\theta$, $\sin\theta$, $\cos\theta$ are located in (i,i), (i,k), (k,i) and (k,k) positions respectively. After making r transformations, we get

$$\begin{aligned} B_r &= S_r^{-1}S_{r-1}^{-1}\cdots S_1^{-1}AS_1\cdots S_{r-1}S_r \\ &= (S_1S_2\cdots S_{r-1}S_r)^{-1}A(S_1S_2\cdots S_{r-1}S_r) \\ &= S^{-1}AS \end{aligned} \tag{6}$$

where $S = S_1S_2\cdots S_{r-1}S_r$.

As $r\to\infty$, B_r approaches a diagonal matrix with the eigenvalues on the leading diagonal. We then have the eigenvectors as the corresponding columns of S. The minimum number of rotations required to bring A into a diagonal form may be $\frac{(n-1)n}{2}$. This procedure, described to reduce the symmetric matrix A to a diagonal matrix D is called the **Jacobi method**.

The method suffers from the following disadvantage:
The elements annihilated by a plane rotation may not necessarily remain zero during subsequent transformations. The value of θ must be checked for its accuracy by checking whether $|\sin^2\theta+\cos^2\theta-1|$, is sufficiently small. The convergence to the eigenvalues takes place even if the pivots are not selected on the basis of their magnitudes, but are selected in the "typewriter fashion".

That is annihilate a_{21}, a_{31}, a_{32}, a_{41}, a_{42}, a_{43} etc. This modification is called the special cyclic Jacobi method. In this method there is no search for the pivots.

Example: Find all the eigenvalues and eigenvectors of the matrix $\begin{bmatrix} 1 & \sqrt{2} & 2 \\ \sqrt{2} & 3 & \sqrt{2} \\ 2 & \sqrt{2} & 1 \end{bmatrix}$.

The largest off diagonal element is $c_{13} = a_{31} = 2$. The other two elements in this 2×2 submatrix are $a_{11} = 1$ and $a_{33} = 1$.
Therefore,
$\theta = \frac{1}{2} \tan^{-1} \left(\frac{4}{0} \right) = \frac{\pi}{4}$.
So,

$$S_1 = \begin{bmatrix} \frac{1}{\sqrt{2}} & 0 & -\frac{1}{\sqrt{2}} \\ 0 & 1 & 0 \\ \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \end{bmatrix}$$

The first rotation gives

$$\begin{aligned} S_1^{-1} A S_1 &= \begin{bmatrix} \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ 0 & 1 & 0 \\ -\frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \end{bmatrix} \begin{bmatrix} 1 & \sqrt{2} & 2 \\ \sqrt{2} & 3 & \sqrt{2} \\ 2 & \sqrt{2} & 1 \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{2}} & 0 & -\frac{1}{\sqrt{2}} \\ 0 & 1 & 0 \\ \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \end{bmatrix} \\ &= \begin{bmatrix} 3 & 2 & 0 \\ 2 & 3 & 0 \\ 0 & 0 & -1 \end{bmatrix} \end{aligned}$$

Again, the largest off diagonal element is $a_{l2} = a_{21} = 2$.
The other elements are an $a_{11} = a_{22} = 3$.
Therefore,
$\theta = \frac{1}{2} \tan^{-1} \left(\frac{4}{0} \right) = \frac{\pi}{4}$.
So,

$$S_2 = \begin{bmatrix} \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

The second rotation gives

$$\begin{aligned} S_2^{-1} A S_2 &= \begin{bmatrix} \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & \sqrt{2} & 2 \\ \sqrt{2} & 3 & \sqrt{2} \\ 2 & \sqrt{2} & 1 \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 1 \end{bmatrix} \\ &= \begin{bmatrix} 5 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix} \end{aligned}$$

Now, we have the matrix of eigenvectors as

$$\begin{aligned} S = S_1 S_2 &= \begin{bmatrix} \frac{1}{\sqrt{2}} & 0 & -\frac{1}{\sqrt{2}} \\ 0 & 1 & 0 \\ \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 1 \end{bmatrix} \\ &= \begin{bmatrix} \frac{1}{2} & -\frac{1}{2} & -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{2} & \frac{1}{2} & -\frac{1}{\sqrt{2}} \end{bmatrix} \end{aligned}$$

Hence, the eigenvalues are $5,\ 1,\ -1$ and the corresponding eigenvectors are the columns of S.

Givens Method for Symmetric Matrices

We have noted that in the Jacobi's method, the elements which were annihilated by a plane rotation may not remain zero during subsequent rotations. Givens proposed an algorithm using plane rotations, which preserves the zeros in the off diagonal elements, once they are created. Let A be a real, symmetric matrix. The Givens method uses the following steps:

(a) reduce A to a tridiagonal form using plane rotations

(b) form a Sturm sequence, study the changes in sign in the sequences and find the eigenvalues

(c) find the eigenvector

The reduction to a tridiagonal form is achieved by using the orthogonal transformations as in the Jacobi method. However, in this case we start with the subspace containing the elements a_{22}, a_{23}, a_{32}, a_{33}. Perform the plane rotation $S_1^{-1}AS_1$ using the orthogonal matrix

$$S_1^* = \begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix} \tag{7}$$

Let the new matrix obtained be $A' = [a'_{ij}]$.

The angle θ is now obtained by putting $a_{13} = a_{31} = 0$ and not by putting $a_{23} = a_{32} = 0$ as in Jacobi method. We find

$$\begin{aligned} a'_{13} &= -a_{12}\sin\theta + a_{13}\cos\theta = 0 \\ \text{or,}\ \tan\theta &= \frac{a_{13}}{a_{12}} \end{aligned} \tag{8}$$

With this value of θ and performing the plane rotation, we produce zeros in the $(3,1)$ and $(1,3)$ positions. Then we perform rotations in $(2,4)$ space and put $a'_{14} = a'_{41} = 0$. This would not affect zeros that have been obtained earlier. Proceeding in this manner, we put $a'_{15} = a'_{51} = 0$ etc. by performing rotations in $(2,5), \cdots, (2,n)$ planes. Then we pass on to the elements $a'_{24}, a'_{25}, \cdots, a_{2n}$ and make them zero by performing rotations in $(3,4), \cdots, (3,n)$ subspaces. Finally, we produce the matrix

$$B = \begin{bmatrix} b_1 & c_1 & & & & \\ c_1 & b_2 & c_2 & & & \\ & c_2 & b_3 & c_3 & & \\ & & & \ddots & & \\ & & & c_{n-2} & b_{n-1} & c_{n-1} \\ & & & & c_{n-1} & b_n \end{bmatrix}$$

The number of plane rotations required to bring a matrix of order n to its tridiagonal form is $\frac{1}{2}(n-1)(n-2)$. We already know that A and B have the same eigenvalues. If $c_i \neq 0$, $i = 1, 2, \cdots, n-1$, then the eigenvalues are distinct. Now, define

$$\begin{aligned} f_n &= |B - \lambda I| \\ &= \begin{vmatrix} b_1-\lambda & c_1 & & & & \\ c_1 & b_2-\lambda & c_2 & & & \\ & c_2 & b_3-\lambda & c_3 & & \\ & & & \ddots & & \\ & & & c_{n-2} & b_{n-1}-\lambda & c_{n-1} \\ & & & & c_{n-1} & b_n-\lambda \end{vmatrix} \end{aligned}$$

Now, expanding by minors, the sequence $\{f_n\}$ satisfies
$f_0 = 1,\ f_1 = \lambda - b_1$
and

$$f_r = (\lambda - b_r)f_{r-1} - c_{r-1}^2 f_{r-2}, \quad 2 \leq r \leq n \tag{9}$$

Note that f_n is the characteristic equation. If none of the $c_1, c_2, \cdots, c_{n-1}$ vanish, then $\{f_n\}$ is a Sturm sequence. That is, if $V(x)$ denotes the number of changes in sign in the sequence for a given number x, then the number of zeros of f_n in $[a, b]$ is $V(a) - V(b)$ (provided a or b is not a zero of f_n). In this way one can approximately compute the eigenvalues and by repeated bisections, one can improve these estimates.

The eigenvectors of B are then found. If these are determined then the eigenvectors of A can be determined, since we know that if v and u are the eigenvectors of B and A respectively, then $u = Sv$, where $S = S_1 S_2 \cdots S_n$ is the product ofthe orthogonal matrices used in the plane rotations. The eigenvectors of B may be found as follows. Neglect a particular equation (say ith) and then solve the remaining equations. This solution usually satisfies the equation that has been left. Then v is the eigenvector determined from these solutions and by putting a zero in the ith position. An advantage of the Givens method is that it takes only a finite number of plane rotations to reduce A to its tridiagonal form.
Example: Use the Givens method to find the eigenvalues of the tridiagonal matrix
$A = \begin{bmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{bmatrix}$.

The Sturm sequence is
$f_0 = 1;\quad f_1 = \lambda - 2;\quad f_2 = (\lambda - 2)f_1 - f_0 = (\lambda-2)^2 - 1;$
$f_3 = (\lambda - 2)f_2 - f_1 = (\lambda - 2)^3 - 2(\lambda - 2)$.

Now, we find

λ	f_0	f_1	f_2	f_3	$V(\lambda)$
-1	$+$	$-$	$+$	$-$	3
0	$+$	$-$	$+$	$-$	3
1	$+$	$-$	0	$+$	2
2	$+$	0	$-$	0	$\cdots$
3	$+$	$+$	0	$-$	1
4	$+$	$+$	$+$	$+$	0

Note that $f_3(2) = 0$, so that $\lambda = 2$ is an eigenvalue. There is an eigenvalue in $(0, 1)$ and $(3, 4)$. We now find better estimates of the eigenvalues by repeated bisections. Let us determine the eigenvalue in $(0, 1)$. We have

λ	f_0	f_1	f_2	f_3	$V(\lambda)$
$\frac{1}{2}$	$+$	$-$	$+$	$-$	3

The eigenvalue is now located in $(0.5, 1)$. Again

λ	f_0	f_1	f_2	f_3	$V(\lambda)$
$\frac{3}{4}$	$+$	$-$	$+$	$+$	2

The eigenvalue is now located in $(0.5, 0.75)$. Then, we have

λ	f_0	f_1	f_2	f_3	$V(\lambda)$
0.625	$+$	$-$	$+$	$+$	2

The eigenvalue is now located in $(0.5, 0.625)$. So, we have

λ	f_0	f_1	f_2	f_3	$V(\lambda)$
0.5625	$+$	$-$	$+$	$-$	3

The eigenvalue is now located in $(0.5625, 0.625)$. Again

λ	f_0	f_1	f_2	f_3	$V(\lambda)$
0.59375	$+$	$-$	$+$	$+$	2

The eigenvalue is now located in $(0.5625, 0.59375)$. We repeat this procedure until the required accuracy is obtained. The exact value of this eigenvalue is $2 - \sqrt{2} \approx 0.585786$.

Finally, we determine the eigenvalue in $(3, 4)$, we have

λ	f_0	f_1	f_2	f_3	$V(\lambda)$
$\frac{7}{2}$	$+$	$+$	$+$	$+$	0

The eigenvalue is now located in $(3, 3.5)$. Again

3.25	$+$	$+$	$+$	$-$	1

The eigenvalue is now located in $(3.25, 3.5)$. Again

$$3.375 \quad + \quad + \quad + \quad - \quad 1$$

The eigenvalue is now located in $(3.375, 3.5)$. Again

$$3.4375 \quad + \quad + \quad + \quad + \quad 0$$

The eigenvalue is now located in $(3.375, 3.4375)$. Again

$$3.40625 \quad + \quad + \quad + \quad - \quad 1$$

The eigenvalue is now located in $(3.40625, 3.4375)$. We repeat this procedure until the required accuracy is obtained. The exact value of this eigenvalue is $2 + \sqrt{2} \approx 3.414213$.

Householder's Method for Symmetric Matrices

We have noticed in the Givens method that the tridiagonalization is achieved by using $\frac{1}{2}(n-1)(n-2)$ plane rotations. However, Householder has given a procedure which requires essentially half as much computation as the Givens method for the tridiagonalization. The remaining procedure is same as in the Givens method. In this method A is reduced to the tridiagonal form by orthogonal transformations representing reflections. The orthogonal transformations are of the form.

$$P = I - 2ww^T \tag{10}$$

where w is a column vector, $w \in R^n$, such that

$$w^T w = w_1^2 + w_2^2 + \cdots + w_n^2 = 1 \tag{11}$$

It can be easily shown that P is symmetric and orthogonal. For that, we have

$$P^T = (I - 2ww^T)^T = I - 2ww^T = P$$

Therefore,

$$\begin{aligned} P^T P &= (I - 2ww^T)(I - 2ww^T) \\ &= I - 4ww^T + 4ww^T ww^T \\ &= I \\ \text{or,} \quad P^T &= P^{-1} \end{aligned}$$

Now, the vectors w are constructed with the first $(r-1)$ components as zeros, that is,

$$w_r^T = (0, 0, \cdots, 0, x_r, x_{r+1}, \cdots, x_n) \tag{12}$$

Since $w_r^T w_r = 1$, so we have $x_r^2 + x_{r+1}^2 + \cdots + x_n^2 = 1$.
Therefore, with this choice of w_r, from the matrices we have

$$P_r = I - 2w_r w_r^T$$

Now, the similarity transformation is given by

$$P_r^{-1} A P_r \;=\; P_r^T A P_r \;=\; P_r A P_r \tag{13}$$

since P_r is symmetric and orthogonal. We put $A = A_1$ and form successively

$$A_r \;=\; P_r A_{r-1} P_r, \quad \text{where } r = 2, 3, \cdots, n-1 \tag{14}$$

At the first transformation, we find x_r's such that we get zeros in the positions $(1,3), (1,4), \cdots, (1,n)$ and in the corresponding positions in the first column. Therefore one rotation brings $n-2$ zeros in the first row and column. In the second rotation, we find x_r's such that we have zeros in $(2,4), (2,5), \cdots, (2,n)$ positions. The final matrix is a tridiagonal matrix as in Given's method. The tridiagonalization is completed with exactly $n-2$ Householder transformations.

Let us illustrate this procedure using a 4×4 matrix

$$A = \begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{bmatrix} \tag{15}$$

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

$$w_2^T \;=\; [0, x_2, x_3, x_4], \quad \text{s.t.} \;\; x_2^2 + x_3^2 + x_4^2 \;=\; 1 \tag{16}$$

Now,

$$P_2 \;=\; I - 2w_2 w_2^T \;=\; \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1-2x_2^2 & -2x_2x_3 & -2x_2x_4 \\ 0 & -2x_2x_3 & 1-2x_3^2 & -2x_3x_4 \\ 0 & -2x_2x_4 & -2x_3x_4 & 1-2x_4^2 \end{bmatrix} \tag{17}$$

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

$$a_{11}, \quad a_{12} - 2p_1x_2, \quad a_{13} - 2p_1x_3, \quad a_{14} - 2p_1x_4, \qquad \text{where } \; p_1 \;=\; a_{12}x_2 + a_{13}x_3 + a_{14}x_4.$$

We now require that

$$a_{13} - 2p_1x_3 \;=\; 0 \tag{18}$$

$$a_{14} - 2p_1x_4 \;=\; 0 \tag{19}$$

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

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

$$\text{or,} \quad a_{12} - 2p_1x_2 \;=\; \pm\sqrt{a_{12}^2 + a_{13}^2 + a_{14}^2} \;=\; \pm s_1 \tag{20}$$

Note that s_1 is a known quantity. Multiply (20) by x_2, (18) by x_3, (19) by x_4 and then adding, we get

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

which gives

$$p_1 = \mp s_1 x_2, \quad \text{since} \quad p_1 = a_{12}x_2 + a_{13}x_3 + a_{14}x_4.$$

Substituting in (20), we get

$$\begin{aligned} a_{12} \pm 2s_1 x_2^2 &= \pm s_1 \\ \pm 2s_1 x_2^2 &= \pm s_1 - a_{12} \\ x_2^2 &= \frac{1}{2}\left(1 \pm \frac{a_{12}}{s_1}\right) \qquad (21) \end{aligned}$$

This determines x_2. From (18) and (19) we have

$$x_3 = \mp \frac{a_{13}}{2s_1 x_2} \qquad (22)$$

$$\text{and} \quad x_4 = \mp \frac{a_{14}}{2s_1 x_2} \qquad (23)$$

Usually, we need to find two square roots, one for and another for x_2. Since x_3 and 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 (21). Choose

$$x_2^2 = \frac{1}{2}\left(1 + \frac{a_{12}\ \text{sign}(a_{12})}{s_1}\right) \qquad (24)$$

The sign of the square root is irrelevent and taken as plus sign. Hence

$$x_3 = \frac{a_{13}\ \text{sign}(a_{12})}{2s_1 x_2}, \quad x_4 = \frac{a_{14}\ \text{sign}(a_{12})}{2s_1 x_2}$$

This transformation produces two zeros in the first row and first column. One more transformation produces zeros in the $(2, 4)$ and $(4, 2)$ positions. The resulting matrix is tridiagonal.

QR method

The QR method is the modification of LR or in particular LU method. So to understand QR method we start from the LR method. **Rutishauser** proposed the LR transformation where L is a lower triangular matrix and R is an upper triangular matrix. In the limit, we get an upper triangular matrix which displays the eigenvalues of A on the leading diagonal. Starting with the matrix $A = A_1$ we split it into two triangular matrices

$$A_1 = L_1 R_1 \qquad (25)$$

with $l_{ii} = 1$, $i = 1, 2, \cdots, n$. Then form $A_2 = R_1 L_1$. Since $A_2 = R_1 L_1 = R_1 A_1 R_1^{-1}$, then A_1 and A_2 have the same eigenvalues. We again write

$$A_2 = L_2 R_2 \qquad (26)$$

with $l_{ii} = 1$, $i = 1, 2, \cdots, n$. Then form $A_3 = R_2 L_2$ so that A_2 and A_3 have the same eigenvalues. Proceeding in this way, we get a sequence of matrices $A_1, A_2, A_3, \cdots$ which in general reduces to an upper triangular matrix. If the eigenvalues are real, then they all lie on the leading diagonal. However, there are difficulties associated with the practical application of the method.

To avoid some of these difficulties, it was proposed that L be replaced by a unitary matrix Q. If A is non-singular then there exists a decomposition $A = QR$ where Q is unitary and R is upper triangular. The QR algorithm is also not simple for practical application. It is useful when applied to a matrix A in upper Hessenberg form (almost triangular form)

$$A = \begin{bmatrix} a_{11} & a_{12} & a13 & \cdots & a_{1,n-1} & a_{1n} \\ a_{21} & a_{22} & a23 & \cdots & a_{2,n-1} & a_{2n} \\ & a_{32} & a33 & \cdots & a_{3,n-1} & a_{3n} \\ \text{O} & & \ddots & \ddots & & \\ & & & & a_{n,n-1} & a_{nn} \end{bmatrix}$$

The number of multiplications and additions in one QR transformation is proportional to n^3 for a full matrix whereas it is only n^2 for a Hessenberg matrix. A two step procedure is recommended, first to reduce A to upper Hessenberg form and then apply QR algorithm to the upper Hessenberg form. Any matrix can be transformed by similarity transformations to the upper Hessenberg form.

Baristow Method

Consider the following polynomial equation of degree n

$$P_n(x) \;=\; x^n + a_1 x^{n-1} + \cdots + a_{n-1}x + a_n \;=\; 0. \tag{27}$$

The Bairstow method extracts a quadratic factor of the form x^2+px+q from the polynomial (27), which may give a pair of complex roots or a pair of real roots. If we divide the polynomial (27) by the quadratic factor x^2+px+q, then we obtain a quotient polynomial $Q_{n-2}(x)$ of degree $n-2$ and a remainder term which is a polynomial of degree one, i.e., $Rx + S$.

Thus

$$P_n(x) \;=\; (x^2+px+q)Q_{n-2}(x) + Rx + S \tag{28}$$

where

$$Q_{n-2}(x) \;=\; x^{n-2} + b_1 x^{n-3} + \cdots + b_{n-3}x + b_{n-2}.$$

The problem is then to find p and q, such that

$$R(p,q) \;=\; 0 \quad \text{and} \quad S(p,q) \;=\; 0. \tag{29}$$

The above equations are two simultaneous equations in two unknowns p and q. Suppose that (p_0, q_0) is an initial approximation and that $(p_0 + \Delta p, q_0 + \Delta q)$ is the true solution.

Following the Newton-Raphson method, we obtain

$$\Delta p = -\frac{RS_q - SR_q}{R_pS_q - R_qS_p} \tag{30}$$

$$\Delta q = -\frac{R_pS - S_pR}{R_pS_q - R_qS_p}, \tag{31}$$

where R_p, R_q, S_p, S_q are the partial derivatives of R and S with respect to p and q evaluated at p_0, q_0.

The coefficients b_i, R and S can be determined by comparing the like powers of x in (28). We obtain

$$\begin{array}{rclrcl}
a_1 &=& b_1 + p & b_1 &=& a_1 - p \\
a_2 &=& b_2 + pb_1 + q & b_2 &=& a_2 - pa_1 - q \\
\vdots & & & \vdots & & \\
a_k &=& b_k + pb_{k-1} + qb_{k-2} & b_k &=& a_k - pa_{k-1} - qa_{n-2} \\
\vdots & & & \vdots & & \\
a_{n-1} &=& R + pb_{n-2} + qb_{n-3} & R &=& a_{n-1} - pb_{n-2} - qb_{n-3} \\
a_n &=& S + qb_{n-2} & S &=& a_n - qb_{n-2}.
\end{array} \tag{32}$$

We now introduce the recursion formula

$$b_k = a_k - pa_{k-1} - qa_{n-2}, \quad k = 1, 2, \cdots, n \tag{33}$$

where $b_0 = 1$ and $b_{-1} = 0$.

Comparing the last two equations with those of (32), we get

$$\begin{array}{rcl} R &=& b_{n-1} \\ S &=& b_n + pb_{n-1} \end{array} \tag{34}$$

The partial derivatives R_p, R_q, S_p and S_q can be determined by differentiating (33) with respect to p and q.

We have

$$-\frac{\partial b_k}{\partial p} = b_{k-1} + p\frac{\partial b_{k-1}}{\partial p} + q\frac{\partial b_{k-2}}{\partial p}, \quad \text{where} \quad \frac{\partial b_0}{\partial p} = \frac{\partial b_{-1}}{\partial p} = 0 \tag{35}$$

$$-\frac{\partial b_k}{\partial q} = b_{k-2} + p\frac{\partial b_{k-1}}{\partial q} + q\frac{\partial b_{k-2}}{\partial q}, \quad \text{where} \quad \frac{\partial b_0}{\partial q} = \frac{\partial b_{-1}}{\partial q} = 0. \tag{36}$$

Now putting

$$\frac{\partial b_k}{\partial p} = -c_{k-1}, \quad k = 1, 2, \cdots, n$$

in the equation (35), we find

$$c_{k-1} = b_{k-1} - pc_{k-2} - qc_{k-3}. \tag{37}$$

Again, if we write

$$\frac{\partial b_k}{\partial p} = -c_{k-2},$$

then the equation (36) gives

$$c_{k-2} = b_{k-2} - pc_{k-3} - qc_{k-4}.$$

Thus, we get a recurrence relation for the determination of c_k from b_k,

$$c_k = b_k - pc_{k-1} - qc_{k-2}, \quad k = 1, 2, \cdots, n-1$$

where $c_0 = 1$ and $c_{-1} = 0$.

We obtain

$$\begin{aligned} R_p &= -c_{n-2}, & S_p &= b_{n-1} - c_{n-1} - pc_{n-2} \\ R_q &= -c_{n-3}, & S_q &= -c_{n-2} - pc_{n-3} \end{aligned}$$

Substituting the above values in (30), (31) and simplifying, we get

$$\begin{aligned} \Delta p &= -\frac{b_n c_{n-3} - b_{n-1} c_{n-2}}{c_{n-2}^2 - c_{n-3}(c_{n-1} - b_{n-1})} \\ \Delta q &= -\frac{b_{n-1}(c_{n-1} - b_{n-1}) - b_n c_{n-2}}{c_{n-2}^2 - c_{n-3}(c_{n-1} - b_{n-1})} \end{aligned}$$

The improved values of p_0 and q_0 are

$$\begin{aligned} p_1 &= p_0 + \Delta p \\ q_1 &= q_0 + \Delta q \end{aligned}$$

Now for computing b_k's and c_k's we use the following scheme:

$$\begin{array}{cccccccc}
 & 1 & a_1 & a_2 & \cdots & a_{n-2} & a_{n-1} & a_n \\
-p & & -p & -pb_1 & \cdots & -pb_{n-3} & -pb_{n-2} & -pb_{n-1} \\
-q & & & -q & \cdots & -qb_{n-4} & -qb_{n-3} & -qb_{n-2} \\
\hline
 & 1 & b_1 & b_2 & \cdots & b_{n-2} & b_{n-1} & b_n \\
-p & & -p & -pc_1 & \cdots & -pc_{n-3} & -pc_{n-2} & \\
-q & & & -q & \cdots & -qc_{n-4} & -qc_{n-3} & \\
\hline
 & 1 & c_1 & c_2 & \cdots & c_{n-2} & c_{n-1} &
\end{array}$$

When p and q have been obtained to the desired accuracy, the polynomial $Q_{n-2}(x) = P_n(x)/(x^2+px+q) = x^{n-2} + b_1 x^{n-4} + \cdots + bn_2$ is called the deflated polynomial. The coefficients $b_i, \quad i = 1, 2, \cdots, n-2$ are known from the synthetic division procedure. The next quadratic factor is obtained using this deflated polynomial.

Example: Perform one iteration of the Bairstow method to extract a quadratic factor $x^2 + px + q$ from the polynomial

$$x^4 + x^3 + 2x^2 + x + 1 = 0$$

using the initial approximations $p_0 = 0.5$, $q_0 = 0.5$.

Solution: Starting with $p_0 = 0.5$ and $q_0 = 0.5$ we obtain

	1	1	2	1	1
-0.5		-0.5	-0.25	-0.625	-0.0625
-0.5			-0.5	-0.25	-0.625
	1	0.5	1.25	$0.125(= b_3)$	$0.3125(= b_4)$
-0.5		-0.5	0.0	-0.375	
-0.5			-0.5	0.0	
	1	$0.0(= c_1)$	$0.75(= c_2)$	$-0.25(= c_3)$	

Therefore

$$\begin{aligned}
\Delta p &= -\frac{b_4 c_1 - b_3 c_2}{c_2^2 - c_1(c_3 - b_3)} = -\frac{0.3125 \times 0.0 - 0.125 \times 0.75}{(0.75)^2 - 0.0(-0.25 - 0.125)} = 0.1667 \\
\Delta q &= -\frac{b_3(c_3 - b_3) - b_4 c_2}{c_2^2 - c_1(c_3 - b_3)} = 0.5
\end{aligned}$$

Hence

$$\begin{aligned}
p_1 &= p_0 + \Delta p = 0.5 + 0.1667 = 0.6667 \\
q_1 &= q_0 + \Delta q = 0.5 + 0.5 = 1
\end{aligned}$$

Thus, the exact values of p and q are 0.6667 and 1.0 respectively.

$\longrightarrow \oplus \longleftarrow$